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Effects of Anthropogenic Hydrocarbon Emission Reductions in Urban Areas with High Biogenic Hydrocarbon Emission Rates: Tampa and St. Petersburg Case Study. LAA Report No. P137-1

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16. ABSTRACT

Literature review and modeling studies were performed to assess the role of biogenic VOC emissions in the photochemical ozone problem of urban areas. The assessment effort focussed specifically on recent research results reported by Georgia Institute of Technology (GIT) scientists indicating that biogenic VOC's in Atlanta reduce substantially the effectiveness of VOC controls in reducing ambient ozone. The GIT findings were checked for accuracy and for consistency with previous studies and also for applicability in other urban areas. EPA and SAI modelers replicated the GIT modeling study and verified its results and conclusions. A conflict between the GIT study and an earlier study by others was resolved, further establishing the validity of the GIT results. Sensitivity studies by EPA modelers showed, however, that the GIT findings, while unquestionably valid for Atlanta, were not necessarily applicable to other urban non-attainment areas. Factors affecting the strength of the biogenic VOC role in the urban ozone problem were found to be the abundance and reactivity of biogenic emissions, the prevailing wind speeds during ozone episodes, the maximum afternoon mixing height, the size of the urbanized area and perhaps other factors also.

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The Role of Biogenic Organics in the Southeast Ozone Problem : Preliminary Assessments and Implications

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Introduction

Photochemical ozone pollution, recognized over three decades ago, has turned out to be one of the most persistent, intractable air pollution problems in the US and other parts of the world[1]. Despite multi-year efforts to reduce emissions of volatile organic compounds (VOC), the ozone air quality standard continues to be violated in over 100 urban areas in the US[2]. Many rural areas also are exposed to elevated ozone concentrations with consequences including costly damage to forests, crops and ecosystems. However, Agency policy has been directed specifically at the urban ozone problem, reflecting the belief that solving the urban ozone problem will also reduce rural ozone. In the Southeast specifically, representatives of States and industrial and scientific communities perceive both the urban and the rural ozone pollution problems as serious. They have been calling for new EPA studies on formation, effects, and control of photochemical ozone in the South, stressing the facts that conditions in the South are particularly conducive for ozone formation and which might reduce effectiveness of O_3 reduction strategies based solely on VOC controls[3].

Several reasons have been hypothesized in the past, for explaining slow progress in alleviating the ozone non-attainment problem in the US cities. Modeling errors due to inaccuracies in the atmospheric chemistry module may have resulted in erroneously low control requirements. Ineffective VOC controls or inadequately enforced control regulations also may have resulted in less control than intended. There is evidence that certain significant manmade VOC emission sources have been overlooked or underestimated, errors which also lead to underestimation of control requirements. It is also conceivable that some controls have reduced the afternoon or evening emissions rather than the morning emissions and have had, therefore, less effect on ozone than if they were distributed equally throughout the day. Another possible reason was added recently when new modeling studies by Trainer _et al_.[4], and by Chameides _et al_.[5], for the Atlanta urban area, indicated that, contrary to previous general understanding, VOC emissions from vegetation might reduce the effectiveness of VOC control substantially in some areas. The preceding factors may have resulted in model-derived control targets that were too low. From the evidence currently in existence, it appears that all of the above factors are credible but their relative importance is neither known nor can it be readily assessed at this time.

EPA is concerned about the Southeast ozone problems and in particular about the role recently attributed to biogenic VOC's in the Atlanta ozone problem. If biogenic VOC emissions have indeed contributed to an underestimation of the level or type of controls needed in Atlanta, as the Chameides et al. study implies, similar effects may have occurred in some other urban areas as well.

Investigating the causes of ozone non-attainment is obviously of highest priority to EPA's Office of Research and Development (ORD) and figures prominently in the ORD's tentative research and development plans for the next several years. The Agency, however, operates currently under severe budget constraints that make it imperative that all research plans first be scrutinized to ensure achievement of those objectives which will have the most benefit. With respect to studies on Southeast ozone issues[3], ORD believes that many of these issues deserve immediate and strong research attention but others are less urgent. The ORD, for example, has judged that at this time ozone effects are of interest only to the extent that they may impact biogenic emission rates; effects-related monitoring studies in the Southeast are not of sufficient priority to justify efforts beyond those in the ORD's base program on ozone effects. ORD is primarily concerned with the methodology for developing appropriate ozone control strategies, and with the role of biogenics in this process, particularly in light of the recent studies in Atlanta.

The Chameides et al. study and its conclusion that biogenic VOC's play an important role in determining effectiveness of strategies to reduce ozone in and near Atlanta need to be evaluated in two respects. First, certain implications of that study make it crucial for the study's results on the effect of biogenic VOC to be quantitatively accurate. Chameides et al. found that when biogenic VOC's were considered, the anthropogenic VOC control requirement for ozone attainment was increased from 30% to as much as 70%, higher than the percent reduction in NO_x needed to achieve the ozone standard. If such a drastic increase in VOC control requirement is indeed correct, it might lead the Agency to judge that NO_x control in addition to VOC control is the preferable approach to ozone reduction. A smaller increase on the other hand might mean that VOC control, although less effective when biogenics are present, is still the preferable approach to ozone reduction. There are several factors that may have affected the accuracy of the Chameides et al. study. Their use of the EKMA model, an EPA-recommended but nonetheless somewhat simplistic model, may have introduced errors resulting from limited treatment of spatial emission patterns and mixing. More importantly, the emission inventory data, particularly those for biogenic VOC, suffer from large uncertainties with regard to both quantity and composition. Treatment of biogenic emissions by current chemical mechanisms also warrants investigation. Finally, there are other, previous studies which appear to contradict that of Chameides at al. for reasons that need to be understood. (See Appendix A).

The other aspect of the Chameides et al. study that needs to be checked is the question of whether the Atlanta findings have broad applicability or reflect Atlanta "uniquenesses". Such uniquenesses, for example, may include an unusual abundance of biogenic VOC's, an unusually reactive biogenic VOC mixture, an unusually favorable combination of weather, anthropogenic and biogenic VOC and NO_x emission conditions, or other unusual factors.

The role of biogenic VOC is probably the most important and pressing question but is not necessarily the only scientific issue related to the Southeast ozone problem. As already stated, the accuracy of the chemistry and dispersion components of the ozone models as well as the accuracy of anthropogenic emission inventory input to the models are factors that are known to impact estimated effects of control strategies and to be subject to substantial errors or uncertainties. Thus, to properly assess the credibility of the ozone control strategies developed for Atlanta and the other Southern cities, it is imperative that errors or uncertainties in the model inputs and the models used to develop those strategies be somehow individually and collectively assessed.

Summarizing, assessment of the causes of non-attainment in Atlanta and other Southern urban areas requires that the issue of the biogenic VOC effect mainly, but some other scientific issues also, in the atmospheric ozone chemistry, meteorology, and modeling areas, should first be resolved. The ozone non-attainment problems in the South appear to deserve special EPA attention both for their own merits and also for their implications with respect to causes of non-attainment in other regions in the country. Before significant resource commitments are made, however, the Agency needs assurances that the evidence pertaining to the need for further studies on the biogenic VOC effect and other aspects of the Southeast ozone problem is credible and conclusive. The research work described and discussed below is an attempt to evaluate such evidence for the purpose of providing the requisite assurances. The intent clearly was to identify and justify future research needs--not to suggest changes in regulatory policy or strategies.

Time and resource constraints dictated that this effort be limited to reviewing published information, and doing quick and simple modeling computations principally using the EKMA or other comparably simple models. The literature review addressed uncertainties in the atmospheric chemistry of biogenic VOC's. One modeling study was conducted for the purpose of completing and re-interpreting an earlier modeling effort to estimate the contribution of biogenic VOC's to the photochemical ozone problem. Another modeling effort was aimed at checking the Chameides et al. modeling computations and exploring the importance of the biogenic VOC factor for a variety of urban emissions and atmospheric conditions representing the diversity of urban areas in the country. Finally, a modeling study was done in which the Atlanta urban plume was modeled using the Airshed grid model. This model, through its detailed inputs, allows us to circumvent some of the concerns about the limited ability of EKMA to treat non-uniformity of emissions and limited mixing. The objectives, research procedures used, and results and conclusions from all those studies are described and discussed in detail in the attached Appendices. In the following section of this report, an attempt is made to summarize all these results and conclusions, to discuss their limitations and, ultimately, to synthesize them into a state-of-science assessment of the biogenic VOC issue and of its implications with respect to the ozone non-attainment problem in the South and other regions of the country.

Summary and Discussion of Results and Conclusions

As discussed above, there are three questions regarding the role of biogenic VOC that need to be addressed. First is the question of whether or not all past and present studies unanimously agree that the role of biogenic VOC in the urban ozone problem is significant. Based on the studies reported here this question can now be answered unequivocally and the answer is given below. The second question deals with the magnitude of the biogenic VOC effect and, specifically, with the degree to which biogenic VOC's increase the VOC emission control requirements for ozone attainment. As discussed below, this question has not been answered completely. Finally, there is the question of whether or not the Chameides et al. results for Atlanta reflect an Atlanta "uniqueness", or, more generally, the question of the degree to which the biogenic VOC effect varies from city to city for the various US non-attainment cities. This question also has not been answered yet for the reasons given below.

Agreement of Studies on Significance of Biogenic VOC Role

The biogenic VOC involvement in the ozone problem has been studied directly, though incompletely, in smog chamber studies and in atmospheric chemistry and modeling studies. When biogenic VOC's were exposed individually or in mixtures to urban atmospheric conditions within smog chambers, they produced significant ozone concentrations, comparable to those produced by anthropogenic VOC's[6,7]. Such substantial ozone-forming potentials for biogenic VOC's are consistent with their ability to react rapidly with the hydroxyl radical (HO)--a reaction that initiates the ozone-forming process--and to produce products many of which also react further to produce ozone. The unanimous current assessment is that existing smog chamber data are consistent with an important role of biogenic VOC's in the urban ozone problem, comparable to the role of the anthropogenic VOC's.

Smog chamber experimentation and evidence, while strongly suggestive, may not be representative of atmospheric conditions, and for that reason are not necessarily conclusive. Although field measurements and evidence would appear to be preferable, the biogenic VOC issue is far too complex to be resolved through field studies alone. One crucial complexity, for example, arises from the rapid destruction of ambient biogenics by HO and O_3 as a result of which only traces of biogenic VOC's are ever measured in the atmosphere[7]. This can misleadingly suggest that such organics cannot possibly have an important role when, in fact, the reacted biogenics are converted into products which react further to produce significant amounts of ozone. To circumvent these limitations of the smog chamber and field data, investigators conceived and applied air quality modeling techniques. Ozone models, when properly validated against theory and smog chamber and field data, are thought to be both credible and useful tools for investigating issues such as the one in hand. One such modeling study was done by Lurmann *et al*. in 1983-84[8] (See also Appendix A). The investigators modeled the Tampa-St. Petersburg urban plume using the ELSTAR photochemical trajectory model, and computed peak ozone concentrations resulting from the anthropogenic VOC emissions alone and from the anthropogenic and biogenic emissions together. Results showed a small ozone increment associated with the inclusion of the biogenic VOC's and were, therefore, interpreted to mean that the biogenic VOC contribution to the urban ozone problem was not significant. Because of apparent conflicts between that study and other newer modeling studies and the smog chamber data, Dr. Lurmann was asked to review his previous work and to re-model the Tampa-St. Petersburg atmosphere in the light of the latest understanding regarding the chemistry and precursor roles in the ozone-forming process. Dr. Lurmann repeated his work using the same model but with an updated chemical mechanism, and the same model inputs, and computed the role of biogenic VOC's as Chameides *et al*. did, that is, in terms of their impact upon the effectiveness of anthropogenic VOC control (See Appendix A). The results from the new study indicated that inclusion of the biogenic VOC's resulted, again, in a small increment in peak ozone concentrations, as found in the earlier study, but the anthropogenic VOC control requirements were substantially increased when biogenic VOC's were included. In one trajectory modeling application, for example, the control requirements in the absence and in the presence of biogenic VOC's were computed to be 70% and 92%, respectively. These numbers do not agree well with the Chameides *et al*. respective numbers of 30% and 100% in an absolute sense. Given, however, that the two studies dealt with different urban areas, and used different models, and drastically different model inputs (e.g. the biogenic VOC emission rate used in the Tampa-St. Petersburg area was only one-half of that used in the Atlanta study), these absolute value disagreements are not significant. What is extremely significant is the agreement between the two studies in that presence of realistic levels of biogenic VOC's can raise the anthropogenic VOC control requirements (for urban ozone attainment) substantially. With this "reconciliation" of the Chameides et al. and Lurmann et al. studies, and in the light of additional corroborating results from the Gipson and SAI studies reported here (see following sections of report and Appendices), it appears that the case for biogenic VOC's having a potentially important role in the design of strategies to reduce the urban ozone problem has been established.

Magnitude of the Biogenic VOC Effect

At first glance, the biogenic VOC effect on urban ozone is understood in terms of the increment in peak ozone concentration that results when biogenic VOC emissions are added to the anthropogenic VOC loading of the urban atmosphere. The Trainer et al.[4] and Chameides et al.[5] studies, however, made it clear that such ozone increments grossly under-reflect the true magnitude of the biogenic VOC effect. Adding VOC emissions, whether anthropogenic or biogenic, to an urban plume raises the VOC-to-NO_x ratio into the domain where peak ozone concentration is insensitive to the VOC precursor factor[1]; that is, increases (or decreases) of VOC emissions will have little impact on ozone. A more meaningful way to define the biogenic VOC effect is in terms of the effect that biogenic VOC's have on the effectiveness of anthropogenic VOC control in reducing ozone. Thus, the biogenic VOC effect as measured by Chameides et al. was to raise the anthropogenic VOC control requirement (for ozone attainment) from 30% to 70% and up to 100%; that is, the biogenic VOC effect was a 40 percentage points increase in the control requirement, and up to 70 percentage points for greater biogenic VOC loadings. Viewed in this context, the biogenic VOC effect, as determined by Chameides et al. for one day in Atlanta, is extremely strong, such that it reduces the effectiveness of VOC control--the traditionally used approach to ozone reduction--to below that of NO_x control. The implications regarding validity of the traditional ozone control strategies are obvious and make it important that the magnitudes of the biogenic VOC effect, as well as of effects from all other factors that impact the relative merits and demerits of the VOC control and NO_x control approaches, be known reliably. This leads to the questions of how accurate is the Chameides et al. study, what are the relative socioeconomic impacts of VOC control and NO_x control, and what other (than on O_3) environmental impacts result from NO_x and VOC controls. It is not within the scope of these short-term studies to answer all these questions comprehensively. Efforts were limited to checking the accuracy of the Chameides et al. study and conclusions only.

To check the accuracy of the Chameides et al. study and conclusions, two efforts were conducted: One by G. Gipson (Appendix B), who duplicated the work by Chameides et al., and also studied the effects of several factors that might have influenced the EKMA modeling results. The second effort was by an SAI contractor (Appendix C) who modeled the same Atlanta urban plume modeled by Chameides et al. and by Gipson, but used the Urban Airshed Model (UAM) in a "low-cost-application mode" (PLANR) instead of EKMA as the modeling tool and somewhat different emissions input. Results from the first part of the Gipson study were in good agreement with those by Chameides et al., a fact that placed added confidence in the calculations done by either investigator. Gipson also repeated his EKMA-Atlanta computations, this time using a somewhat adjusted technique and inputs to reflect the latest EPA guidance (on use of EKMA) and Atlanta-SIP information but using the Chameides et al. estimate of biogenic VOC emissions. Results showed the VOC control requirement to increase from 31% to 86% when biogenic VOC's were included. Results from the low-cost-applications of the UAM model were that inclusion of biogenic VOC's raised the anthropogenic VOC control requirement from 62% to 100%, that is, by 38 percentage points, compared to 30%-to-70% or 40 percentage points from the Chameides et al. study and 31%-to-86% or 55 percentage points from the Gipson study. The three studies agree that the control requirement change is large but they disagreed somewhat on the magnitude of the change and strongly on the absolute values. The following discussion deals with some of the factors responsible for these disagreements.

There are several factors of uncertain magnitude that can cast doubts on the modeling estimates of the role of biogenic VOC. First, there is the "model uncertainty" factor which, judging from the differences among the UAM and EKMA control requirement predictions reported here, and from current judgment, in general, concerning the validity and accuracy of current ozone models[9], will have to be considered as an important one. Thus, the simplifications underlying the EKMA concept and those associated with the PLANR use of the UAM model, could be sources of potentially large errors. Other relevant factors are the biogenic VOC emissions level, composition and atmospheric chemistry accuracy factors, of which the first was studied by Chameides et al. and by Gipson (Appendix B) and found to be important. The importance of accuracy of biogenic VOC composition and of atmospheric chemistry as factors affecting the biogenic VOC role has not been specifically and adequately studied. Given, however, the substantial differences in reactivity with the hydroxyl radical (HO) and in atmospheric reaction product composition among different biogenic VOC's, these factors should be important (See Appendix D also). Finally, there are other important factors some of which were explored in sensitivity analyses done by Gipson, as a part of his EKMA study (Appendix B), and by SAI, as part of their PLANR-UAM study (Appendix C). Most significant findings from these analyses were that EKMA-estimates of the biogenic VOC effect differ widely for different biogenic VOC levels, for different ozone episodes modeled, and for different atmospheric dilutions (i.e. different maximum afternoon mixing heights). Also, UAM results were sensitive to wind speeds. Their findings suggested, for example, that given the large differences in biogenic VOC emission levels between center-city and outlying sections of urban areas, it may be important to use emission rate data with a high degree of spatial resolution rather than more coarsely resolved data (e.g. county- wide average values).

The conclusion from all the studies and theoretical analyses discussed above is that the magnitude of the biogenic VOC effect, while unquestionably significant, cannot be quantified with confidence at this time. It cannot be determined reliably for each and every non-attainment urban area whether the biogenic VOC effect is large enough to justify use of additional VOC control or adoption of vigorous concurrent NO_x controls along with VOC controls as the most effective approach to ozone attainment. Before final judgments can be made, (1) model accuracy must be assessed and, if necessary, further improved, and (2) model inputs, especially the levels, composition and atmospheric chemistry of biogenic VOC's mainly, but of anthropogenic VOC's also, must be determined more reliably and with the requisite spatial and temporal detail. Using such improved methodologies and data, the biogenic VOC role should then be determined for each non-attainment area separately, through modeling/field studies of several ozone episodes and with accurate measurements of the boundary conditions and atmospheric dilution (mixing height) and transport factors.

Uniquenesses of Atlanta Ozone Problem

While there can be little doubt at this point that biogenic VOC's reduce significantly the effectiveness of anthropogenic VOC controls alone in Atlanta, this may or may not be the case for each and every non-attainment urban area. To explore this possibility, Gipson performed a sensitivity analysis to determine the degrees to which factors that vary from city to city affect EKMA computations of the biogenic VOC role (Appendix B). Specific factors that were thought to be important and were included in the study were the biogenic VOC abundance and composition and the number of hours the urban plume travels above the urbanized area. This latter factor reflects wind speed conditions or size of the urban area.

Biogenic VOC inventory and composition data for Atlanta and other urban areas have been compiled by EPA[10] for use with EPA's gridded (1/4 longitude x 1/6 latitude or, roughly, 20 Km x 20 Km grid size) Regional Ozone Model (ROM). Based on these data, the Atlanta downtown cell is shown to have a daily emission loading of 3 Kg/Km^2 for isoprene and 8 Kg/Km^2 for total biogenic VOC, during a day with clear skies and 99°F maximum temperature. These loadings are much smaller than the respective 30 Kg/Km^2 and 50 Kg/Km^2 loadings used by Chameides *et al*., but the Chameides *et al*. data compare reasonably well with the loadings in the outlying grid cells. If atmospheric stagnation conditions are such that the

Atlanta peak ozone concentration occurs while the urban plume is still within the urbanized section of the Atlanta area, then EKMA calculations show the biogenic VOC's to increase the VOC control requirement from 31% to 38%, that is, only by 7 percentage points, compared to the 40 percentage points computed by Chameides et al. Such a strong stagnation situation in Atlanta may, of course, be only hypothetical. It is mentioned here primarily for the purpose of illustrating that under different conditions the biogenic VOC effect could conceivably be much smaller than that indicated by the Chameides et al. results. This situation is not totally unrealistic. It can occur, for example, in urban areas with unusually large "urbanized sections" (e.g. Los Angeles, New York City), such that the ozone peaks before the urban plume exits into the outlying vegetated areas.

Comparison of the Atlanta biogenic emissions loadings with those of other urban areas, shows that Atlanta is somewhat unusual in that its biogenic VOC factor is relatively strong. Thus, using the ROM emission inventory data discussed above, it can be shown that Atlanta, and especially Baton Rouge, have higher biogenic VOC loadings, than those in Houston, Philadelphia, New York City, Baltimore, and Pittsburgh, by as much as an order of magnitude in some cases. Furthermore, the content of the extremely reactive isoprene ranges widely, roughly from 10% to 50% of total biogenic VOC, with Atlanta probably lying near the high end of the range.

It can be concluded from the above that the biogenic VOC factor for some urban areas may be as strong or stronger than in Atlanta but for other cities it may be considerably less important. Evidently, each urban area should be evaluated separately, based on its own biogenic VOC emissions loading factor, the biogenic VOC composition, the size of its "urbanized section", the prevailing wind speeds during ozone episodes, the maximum afternoon mixing height, and perhaps other factors also.

Current Assessment of Biogenic VOC Factor. Recommendations for New Research

The preceding analysis of currently existing evidence led to the following assessment of the biogenic VOC role and associated implications.

- Biogenic VOC's in Atlanta are more important than previously believed.

- "Importance" in other cities varies, possibly widely. Atlanta may be relatively unique due to unusually high biogenic VOC emissions (e.g. higher than in Houston, Baltimore, New York, Philadelphia) as well as a highly reactive mix of biogenic emissions.

- Much uncertainty exists in quantitative estimates of the biogenic VOC role because of limited data on levels, composition and atmospheric chemistry of biogenic VOC emissions, e.g.
    - Biogenic VOC emissions depend strongly on temperature, sunlight, vegetation species, foliage and land use, factors which either are not well known or are not well understood.
    - Atmospheric chemistry is little understood for isoprene and even less for the other biogenic VOC's.
- VOC control requirements in the past were probably underestimated because of lack of data on, or underestimation of, the biogenic VOC role.
- NO_x emissions may be more important than previously believed in areas high in biogenic VOC emissions.

The findings from this assessment suggest that the biogenic VOC factor is sufficiently important to warrant further research. Specific new research programs called for are:

- Case studies of ozone non-attainment in Atlanta and other Southern and Northern urban areas;
- Emissions studies of biogenic and anthropogenic VOC's;
- Atmospheric chemistry and model development studies; and
- Monitoring studies for problem diagnosis purposes.

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Appendices

A. "The Effects of Anthropogenic Hydrocarbon Emission Reductions in Urban Areas with High Biogenic Hydrocarbon Emission Rates: Tampa/St. Petersburg Case Study", by F. Lurmann, Lurmann & Associates, Santa Barbara, CA, March 1989.

B. "Sensitivity of EKMA Model Predictions to Biogenic Emissions", by G. L. Gipson, EPA/ORD/AREAL, Research Triangle Park, NC 27711, April 1989.

C. "Low-Cost Application of the Urban Airshed Model to Atlanta and Evaluation of the Effects of Biogenic Emissions on Emission Control Strategies", by R. E. Morris, T. C. Myers, M. C. Causley and L. A. Cardner. Interim Report, Contract 68-02-4352, Systems Applications, Inc., April 1989.

D. "Biogenic VOC Uncertainties", by J. Bufalini, EPA/ORD/AREAL, Research Triangle Park, NC 27711, March 1989.

APPENDIX A

The Effects of Anthropogenic Hydrocarbon Emission Reductions in Urban Areas With High Biogenic Hydrocarbon Emission Rates: Tampa/St. Petersburg Case Study

March 1989

Lurmann & Associates
Santa Barbara, CA

THE EFFECTS OF ANTHROPOGENIC HYDROCARBON EMISSION REDUCTIONS IN URBAN AREAS WITH HIGH BIOGENIC HYDROCARBON EMISSION RATES: TAMPA/ST. PETERSBURG CASE STUDY

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1. INTRODUCTION

Approximately seventy urban areas in the United States failed to meet the Clean Air Act's 1987 deadline for compliance with the National Ambient Air Quality Standard (NAAQS) for ozone. The widespread failure to meet this goal suggests that there may be serious deficiencies in the methods used to design and/or implement ozone control strategies. There are many potential causes of this problem. Some of the more likely causes are the reliance on simplistic atmospheric models, inadequate aerometric and emissions data bases, overly optimistic assumptions for the effectiveness of control measures and their rates of implementation, and underestimation of the effects of long range transport. Deficiencies in the data bases and models also may have lead to strategies that relied on hydrocarbon[1] (HC) reductions alone, rather NO_x or HC and NO_x strategies which may be more effective in certain areas.

One factor that may have contributed to the problem is underestimation of the baseline emissions inventories. Underestimation of reactive organic emissions can lead to underestimation of the amount of emission reductions needed to achieve compliance with the standard. Certain categories of anthropogenic hydrocarbon (AHC) emissions (e.g. hot running evaporative emissions from gasoline vehicles) and virtually all biogenic hydrocarbon (BHC) were omitted in the atmospheric modeling used to develop ozone control strategies in the early 1980s. The U.S. Environmental Protection Agency's (EPA) current guidelines do not require inclusion of biogenic emissions in the emissions inventories used for SIP ozone modeling. Recent work by Chameides et al. (1988) for Atlanta, Georgia suggests that biogenic hydrocarbons can have a

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[1] Throughout this report the term hydrocarbon refers to both hydrocarbon and oxygenated organic compounds.

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substantial effect on the design of ozone control strategies. They found that when a 50 kg/km^2/day emission rate for isoprene was included in the simulations, the anthropogenic HC emission control requirement needed to meet the standard increased from 30% to 100%. They also found that when biogenic HC emission rates greater than 30 kg/km^2/day were included, the ozone standard could be achieved with smaller percentage reductions in NO_x emissions than in anthropogenic HC emissions. These results may have important technical and policy implications, and warrant further investigation.

The purpose of the present study is to investigate the effects of anthropogenic HC reductions in urban areas that have substantial biogenic HC emissions and to determine if the Chameides et al. findings apply to other areas. The Tampa/St. Petersburg, Florida region is well suited to investigation of this subject because half of the HC emissions in this area are estimated to be emitted by vegetation, and approximate temporal and spatial distributions of the biogenic emissions have been compiled.

The approach adopted for this study is to use the ELSTAR photochemical trajectory model and the modeling data base that was set up to assess the contribution of biogenic emissions to ambient ozone concentrations in the Tampa/St. Petersburg area by Lurmann et al. (1984). The data base was produced in EPA sponsored studies in the 1970s to collect aerometric data and compile both anthropogenic and biogenic emission inventories for this area (Wayne and Kochis 1978; Zimmerman 1979). The present study is designed to begin where the modeling study of Lurmann et al. (1984) ended and address important questions that were not considered in that study. Both the original and an updated photochemical model are used to investigate the effects of substantial anthropogenic emission reductions in the Tampa/St. Petersburg area. The modeling results are used to assess the importance of including biogenic emissions in the modeling used to formulate ozone control strategies.

2. THE AIR QUALITY MODEL

The ELSTAR air quality model is a fixed-width single column multi-layer photochemical trajectory model which has been tested against ambient data in St. Louis (Shreffler and Schere 1982) and Los Angeles (Lloyd et al 1979). Two versions of the ELSTAR air quality model are employed in this study. The first version, referred to as the "original model", incorporate the anthropogenic HC/NO_x chemical mechanism of Atkinson et al. (1982) and the biogenic HC chemical mechanism of Lloyd et al. (1983). The second version, referred to as the "updated model", incorporates the chemical mechanism shown in Tables 1 through 3. The updated model's chemical mechanism is a version of the condensed mechanism for anthropogenic HC species reported by Lurmann et al. (1987) that incorporates the recent recommendations of DeMore et al. (1988) and Atkinson (1988) for kinetic parameters. This mechanism also includes an updated version of the Lloyd et al. (1983) chemical mechanism for isoprene and α-pinene. The updated anthropogenic HC/NO_x mechanism has virtually the same lumped organic precursor species and surrogate species as included in the Atkinson et al. (1982) mechanism (ie., lumped >C3 alkanes, ethene, propene, trans-2-butene, toluene, lumped higher aromatics, formaldehyde, and acetaldehyde), however, it is based on more recent kinetic and mechanistic data, and it has been tested much more extensively against environmental chamber data (Carter et al. 1986; Lurmann et al. 1987, Carter 1988). The updated isoprene mechanism incorporates new rate constants for the reactions of isoprene, methyl vinyl ketones, and mathacrolein, and various changes to make the mechanism consistent with the assumptions used for the other alkene reactions in the Lurmann et al. (1987) mechanism. It does not incorporate results from recent OH reaction product studies that show some of the products are different than assumed in the Lloyd et al. mechanism and that about half of the carbon from the isoprene and mathacrolein reactions with OH is contained in species that have not been identified (Gu et al. 1985; Atkinson et al. 1989a,1989b; Tuazon and Atkinson 1989). Updating the products and parameterizing the effects of the unknown species using chamber data was beyond the scope of this study. Clearly, it should be recognized that the chemical mechanisms employed herein for isoprene and α-pinene are highly uncertain.

It is also important to recognize that trajectory models are inherently limited in their ability to simulated complex air flow patterns and multi-day air flow patterns. A trajectory model is used here primarily for the sake of convenience (since it was already set-up in the previous study). The type of flow patterns that occur in coastal areas like Tampa and St. Petersburg justify using an Eulerian modeling approach. We expect the trajectory model and an Eulerian model would respond in qualitatively similar manners to the "bounding type" of emission scenarios considered herein. However, the importance of transport should not be treated lightly in studies of the effects of biogenic hydrocarbons because the biogenic hydrocarbons must be accurately transported to the regions with NO_x emissions in order to accurately estimate their effects on ozone.

Table 1. The chemical reaction mechanism for the updated model.

	REACTION	RATE CONSTANTS AT 298 K & 1 ATM		
		$PPM^{-1}MIN^{-1}$	$CM^3MOLEC^{-1}SEC^{-1}$	-E/R
1.	NO2 + hv ---> NO + O	See Table 2		
2.	O ---> O3	4.605E+06	7.676E+04	
3.	O + NO2 ---> NO	1.436E+04	9.721E-12	-7300
4.	O + NO2 ---> NO3	2.363E+03	1.600E-12	120
5.	NO + O3 ---> NO2	2.686E+01	1.818E-14	
6.	NO2 + O3 ---> NO3	4.784E-02	3.239E-17	-1370
7.	NO + NO3 ---> 2.NO2	4.153E+04	2.812E-11	-2450
8.	NO + NO ---> 2.NO2	1.428E-04	9.669E-20	150
9.	NO2 + NO3 ---> N2O5	1.726E+03	1.168E-12	529
10.	N2O5 ---> NO2 + NO3	2.151E+00	3.585E-02	246
11.	N2O5 + H2O ---> 2.HNO3	1.477E-06	1.000E-21	-11108
12.	NO2 + NO3 ---> NO + NO2	5.986E-01	4.053E-16	-1229
13.	NO3 + hv ---> NO	See Table 2		
14.	NO3 + hv ---> NO2 + O	See Table 2		
15.	O3 + hv ---> O	See Table 2		
16.	O3 + hv ---> O*SD	See Table 2		
17.	O*SD + H2O ---> 2.OH	3.249E+05	2.200E-10	
18.	O*SD ---> O	4.320E+10	7.200E+08	
19.	NO + OH ---> HONO	7.267E+03	4.920E-12	670
20.	HONO + hv ---> NO + OH	See Table 2		
21.	NO2 + H2O ---> HONO - NO2 + HNO3	1.477E-09	1.000E-24	
22.	NO2 + OH ---> HNO3	1.708E+04	1.156E-11	617
23.	HNO3 + hv ---> NO2 + OH	See Table 2		
24.	HNO3 + OH ---> NO3	1.887E+02	1.278E-13	778
25.	CO + OH ---> HO2	3.545E+02	2.400E-13	
26.	O3 + OH ---> HO2	1.003E+02	6.792E-14	-942
27.	NO + HO2 ---> NO2 + OH	1.222E+04	8.275E-12	240
28.	HO2 + NO2 ---> HNO4	2.042E+03	1.383E-12	632
29.	HNO4 ---> HO2 + NO2	5.101E+00	8.502E-02	-10244
30.	HNO4 + hv ---> HO2 + NO2	See Table 2		
31.	HNO4 + OH ---> NO2	6.868E+03	4.650E-12	380
32.	O3 + HO2 ---> OH	3.017E+00	2.043E-15	-502
33.	HO2 + HO2 ---> H2O2	4.593E+03	3.110E-12	619
34.	HO2 + HO2 + H2O ---> H2O2	2.314E-01	6.364E-30	2818
35.	H2O2 + hv ---> 2.OH	See Table 2		
36.	H2O2 + OH ---> HO2	2.492E+03	1.687E-12	-200
37.	NO3 + HO2 ---> HNO3	4.593E+03	3.110E-12	619
38.	NO3 + HO2 + H2O ---> HNO3	2.314E-01	6.364E-30	2818
39.	OH + HO2 --->	1.469E+05	9.949E-11	230
40.	RO2 + NO ---> NO	1.135E+04	7.681E-12	180
41.	RO2 + HO2 ---> HO2	7.397E+03	5.008E-12	1000
42.	RO2 + RO2 --->	1.477E+00	1.000E-15	
43.	RO2 + RCO3 --->	4.431E+03	3.000E-12	
44.	RCO3 + NO ---> NO	1.135E+04	7.681E-12	180
45.	RCO3 + NO2 ---> NO2	6.753E+03	4.572E-12	180
46.	RCO3 + HO2 ---> HO2	7.397E+03	5.008E-12	1000
47.	RCO3 + RCO3 --->	7.828E+03	5.300E-12	
48.	ROOH + hv ---> HO2 + OH	See Table 2		
49.	ROOH + OH ---> .5RO2R + .5OH + .5RO2	1.081E+04	7.316E-12	180

Table 1 (continued).

	REACTION	RATE CONSTANTS AT 298 K & 1 ATM		
		$\text{PPM}^{-1}\text{MIN}^{-1}$	$\text{CM}^{3}\text{MOLEC}^{-1}\text{SEC}^{-1}$	-E/R
50.	HCHO + hv ---> 2.HO2 + CO	See Table 2		
51.	HCHO + hv ---> CO	See Table 2		
52.	HCHO + OH ---> HO2 + CO	1.634E+04	1.106E-11	-110
53.	HCHO + NO3 ---> HNO3 + HO2 + CO	8.887E-01	6.017E-16	-2518
54.	HCHO + HO2 ---> RO2R + RO2	1.477E+00	1.000E-15	
55.	ALD2 + OH ---> MCO3 + RCO3	2.347E+04	1.589E-11	311
56.	ALD2 + hv ---> CO + HCHO + HO2 + RO2R + RO2	See Table 2		
57.	ALD2 + NO3 ---> HNO3 + MCO3 + RCO3	3.944E+00	2.671E-15	-1867
58.	MCO3 + NO ---> NO2 + HCHO + RO2R + RO2	1.135E+04	7.681E-12	180
59.	MCO3 + NO2 ---> PAN	6.753E+03	4.572E-12	180
60.	MCO3 + HO2 ---> ROOH + HCHO	7.397E+03	5.008E-12	1000
61.	MCO3 + RO2 ---> .5HO2 + HCHO + RO2	4.431E+03	3.000E-12	
62.	MCO3 + RCO3 ---> HO2 + HCHO + RCO3	7.828E+03	5.300E-12	
63.	PAN ---> MCO3 + NO2 + RCO3	2.257E-02	3.761E-04	-13542
64.	MEK + hv ---> ALD2 + MCO3 + RO2R + RO2 + RCO3	See Table 2		
65.	MEK + OH ---> .5ALD2 + .5HCHO + MCO3 + 1.5RO2R + 1.5RO2 + RCO3	1.457E+03	9.863E-13	-745
66.	MGLY + hv ---> MCO3 + HO2 + CO + RCO3	See Table 2		
67.	MGLY + OH ---> MCO3 + CO + RCO3	2.511E+04	1.700E-11	
68.	MGLY + NO3 ---> HNO3 + MCO3 + CO + RCO3	3.697E+00	2.503E-15	-1427
69.	CH4 + OH ---> HCHO + RO2R + RO2	1.145E+01	7.751E-15	-1710
70.	ALKA + OH ---> .111HCHO + .53ALD2 + .64MEK + .13RO2N + .87RO2R + .7R2O2 + 1.7RO2	6.735E+03	4.560E-12	
71.	RNO3 + OH ---> NO2 + .15MEK +1.53ALD2 + .16HCHO +1.39R2O2 +1.39RO2	3.000E+03	2.031E-12	-709
72.	RO2N + NO ---> RNO3	1.135E+04	7.681E-12	180
73.	RO2N + HO2 ---> ROOH + MEK	7.397E+03	5.008E-12	1000
74.	RO2N + RO2 ---> RO2 + .5HO2 + MEK	1.477E+00	1.000E-15	
75.	RO2N + RCO3 ---> RCO3 + HCHO + HO2 + MEK	4.431E+03	3.000E-12	
76.	R2O2 + NO ---> NO2	1.135E+04	7.681E-12	180
77.	R2O2 + HO2 ---> ROOH	7.397E+03	5.008E-12	1000
78.	R2O2 + RO2 ---> RO2	1.477E+00	1.000E-15	
79.	R2O2 + RCO3 ---> RCO3 + HCHO + HO2	4.431E+03	3.000E-12	
80.	RO2R + NO ---> NO2 + HO2	1.135E+04	7.681E-12	180
81.	RO2R + HO2 ---> ROOH	7.397E+03	5.008E-12	1000
82.	RO2R + RO2 ---> .5HO2 + RO2	1.477E+00	1.000E-15	
83.	RO2R + RCO3 ---> RCO3 + HCHO + HO2	4.431E+03	3.000E-12	
84.	ETHE + OH ---> 1.56HCHO + .22ALD2 + RO2R + RO2	1.260E+04	8.533E-12	411
85.	ETHE + O3 ---> HCHO + .12HO2 + .42CO + .4CRG1	2.581E-03	1.747E-18	-2634
86.	ETHE + O ---> HCHO + HO2 + CO + RO2R + RO2	1.078E+03	7.301E-13	-792
87.	ETHE + NO3 ---> NO2 + 2.HCHO + R2O2 + RO2	2.999E-01	2.030E-16	-2925
88.	PRPE + OH ---> RO2R + HCHO + ALD2 + RO2	3.884E+04	2.630E-11	504
89.	PRPE + O3 ---> .64HCHO + .5ALD2 + .28CO + .06OH + .17HO2 + .13RO2R + .13RO2 + .2CRG1 + .1CRG1	1.674E-02	1.133E-17	-2105
90.	PRPE + O ---> .2MEK + .4HCHO + .2ALD2 + .2HO2 + .6RO2R + .4CO + .6RO2	5.879E+03	3.980E-12	-324
91.	PRPE + NO3 ---> NO2 + HCHO + ALD2 + R2O2 + RO2	1.121E+01	7.593E-15	-1935

Table 1 (continued).

	REACTION			RATE CONSTANTS AT 298 K & 1 ATM		
				PPM^{-1}MIN^{-1}	CM^{3}MOLEC^{-1}SEC^{-1}	-E/R
92.	TBUT + OH	--->	RO2R + 2.ALD2 + RO2	9.406E+04	6.368E-11	549
93.	TBUT + O3	--->	ALD2 + .15CO + .27RO2R + .12OH + .21HO2 + .27RO2 + .30HCHO + .2CRG2	2.960E-01	2.004E-16	-1137
94.	TBUT + O	--->	MEK + .4HO2	3.452E+04	2.337E-11	10
95.	TBUT + NO3	--->	NO2 + 2.ALD2 + R2O2 + RO2	5.613E+02	3.800E-13	-975
96.	CRG1 + NO	--->	NO2 + HCHO	1.135E+04	7.681E-12	180
97.	CRG1 + NO2	--->	NO3 + HCHO	1.135E+03	7.681E-13	180
98.	CRG1 + H2O	--->	FRMA	3.397E-02	2.300E-17	
99.	CRG2 + NO	--->	NO2 + ALD2	1.135E+04	7.681E-12	180
100.	CRG2 + NO2	--->	NO3 + ALD2	1.135E+03	7.681E-13	180
101.	CRG2 + H2O	--->	ACTA	3.397E-02	2.300E-17	
102.	CRG1 + HCHO	--->	OZID	3.693E+01	2.500E-14	
103.	CRG2 + HCHO	--->	OZID	3.693E+01	2.500E-14	
104.	CRG1 + ALD2	--->	OZID	3.693E+01	2.500E-14	
105.	CRG2 + ALD2	--->	OZID	3.693E+01	2.500E-14	
106.	TOLU + OH	--->	.16CRES + .16HO2 + .84RO2R + .40DIAL + .84RO2 + .14MGLY + .11HCHO + .11CO	9.134E+03	6.184E-12	322
107.	AROM + OH	--->	.17CRES + .17HO2 + .83RO2R + .83RO2 + .59DIAL + .52MGLY + .06HCHO + .06CO	5.819E+04	3.940E-11	
108.	DIAL + OH	--->	MCO3 + RCO3	4.431E+04	3.000E-11	
109.	DIAL + hv	--->	HO2 + CO + MCO3 + RCO3	See Table 2		
110.	CRES + OH	--->	.2MGLY + .15RO2N + .85RO2R + RO2 + .08CRES	5.908E+04	4.000E-11	
111.	CRES + NO3	--->	HNO3 + BZO + .5CRES	3.249E+04	2.200E-11	
112.	BZO + NO2	--->	RNO3	2.216E+04	1.500E-11	
113.	BZO + HO2	--->		7.397E+03	5.008E-12	1000
114.	BZO	--->		6.000E-02	1.000E-03	
115.	OH + ISOP	--->	RO2R + RO2 + HCHO + .5MVK + .5MACR	1.484E+05	1.005E-10	410
116.	OH + MVK	--->	.67R2O2 + .67MCO3 + .67HAC + .33HCHO + .33RO2R + .33MGLY + RO2 + .67RCO3	2.778E+04	1.881E-11	452
117.	MACR + OH	--->	MAO3 + RCO3 + H2O	1.647E+04	1.115E-11	175
118.	MAO3 + NO2	--->	MPAN	6.753E+03	4.572E-12	180
119.	MPAN	--->	MAO3 + NO2 + RCO3	2.249E-02	3.749E-04	-13543
120.	MAO3 + NO	--->	NO2 + HO2 + MGLY + 2.R2O2 + 2.RO2	1.135E+04	7.681E-12	180
121.	MAO3 + HO2	--->	ROOH + MGLY	7.397E+03	5.008E-12	1000
122.	MAO3 + RO2	--->	.5HO2 + MGLY + RO2	4.431E+03	3.000E-12	
123.	MAO3 + RCO3	--->	HO2 + MGLY + RCO3	7.828E+03	5.300E-12	
124.	MACR + OH	--->	RO2R + HCHO + MGLY + RO2	3.294E+04	2.230E-11	175
125.	HAC + hv	--->	HCHO + 2.HO2 + CO	See Table 2		
126.	HAC + OH	--->	MCO3 + RCO3	2.216E+04	1.500E-11	
127.	O3 + ISOP	--->	.5HCHO + .2MVK + .3MACR + .2CRG1 + .06HO2 + .2CO + .2MVKO + .3MACO	2.117E-02	1.433E-17	-2014
128.	O3 + MVK	--->	.5HCHO + .2CRG1 + .21HO2 + .2MGLO + .2CO + .15ALD2 + .15MCO3 + .15RCO3	7.365E-03	4.986E-18	-2014
129.	O3 + MACR	--->	.65HCHO + .2CRG1 + .5MGLY + .2MGLO + .36HO2 + .35CO + .15R2O2 + .15RO2	1.682E-03	1.139E-18	-2518
130.	MVKO + NO	--->	MVK + NO2	1.135E+04	7.681E-12	180
131.	MVKO + NO2	--->	MVK + NO3	1.135E+03	7.681E-13	180
132.	MVKO + H2O	--->	PROD	3.397E-02	2.300E-17	

Table 1 (continued).

	REACTION			RATE CONSTANTS AT 298 K & 1 ATM		
				$PPM^{-1}MIN^{-1}$	$CM^{3}MOLEC^{-1}SEC^{-1}$	-E/R
133.	MACO + NO	--->	MACR + NO2	1.135E+04	7.681E-12	180
134.	MACO + NO2	--->	MACR + NO3	1.135E+03	7.681E-13	180
135.	MACO + H2O	--->	PROD	3.397E-02	2.300E-17	
136.	MGLO + NO	--->	MGLY + NO2	1.135E+04	7.681E-12	180
137.	MGLO + NO2	--->	MGLY + NO3	1.135E+03	7.681E-13	180
138.	MGLO + H2O	--->	PROD	3.397E-02	2.300E-17	
139.	ISOP + NO3	--->	NO2 + HCHO + .5MVK + .5MACR + R2O2 + RO2	1.999E+03	1.082E-12	-942
140.	MVK + NO3	--->	NO2 + HCHO + .5MCO3 + .5MGLY + R2O2 + .5HO2 + .5RCO3 + RO2	1.477E-01	1.000E-16	
141.	MACR + NO3	--->	NO2 + HCHO + .5MGLY + R2O2 + RO2	4.038E+00	2.734E-15	-1860
142.	OH + PIN	--->	PCHO + RO2R + RO2	8.217E+04	5.564E-11	500
143.	PCHO + hv	--->	ALD2 + HO2 + RO2R + RO2	See Table 2		
144.	PCHO + hv	--->	ALD2 + MVK	See Table 2		
145.	OH + PCHO	--->	PCO3 + RCO3	2.216E+04	1.500E-11	
146.	PCO3 + NO2	--->	PIAN	6.753E+03	4.572E-12	180
147.	PIAN	--->	PCO3 + NO2 + RCO3	2.249E-02	3.749E-04	-13543
148.	PCO3 + NO	--->	NO2 + ALD2 + R2O2 + RO2	1.135E+04	7.681E-12	180
149.	PCO3 + HO2	--->	ROOH + ALD2	7.397E-02	5.008E-17	1000
150.	PCO3 + RO2	--->	.5HO2 + ALD2 + RO2	4.431E+03	3.000E-12	
151.	PCO3 + RCO3	--->	HO2 + ALD2 + RCO3	7.828E+03	5.300E-12	
152.	O3 + PIN	--->	BIR	1.255E-01	8.496E-17	-1170
153.	BIR + NO	--->	PCHO + NO2	1.135E+04	7.681E-12	180
154.	BIR + NO2	--->	PCHO + NO3	1.135E+03	7.681E-13	180
155.	BIR + H2O	--->	PROD	2.511E-03	1.700E-18	

Table 2. Photolytic reaction rates (per minute) for the updated mechanism.

	Solar Zenith Angle (degress)									
Reaction No.	0	10	20	30	40	50	60	70	78	86
1	.5554E+00	.5515E+00	.5396E+00	.5171E+00	.4837E+00	.4315E+00	.3539E+00	.2389E+00	.1209E+00	.2458E-01
13	.1157E+01	.1154E+01	.1143E+01	.1122E+01	.1091E+01	.1039E+01	.9495E+00	.7739E+00	.4847E+00	.7616E-01
14	.1049E+02	.1044E+02	.1034E+02	.1013E+02	.9828E+01	.9299E+01	.8415E+01	.6722E+01	.4072E+01	.6311E+00
15	.3121E-01	.3106E-01	.3062E-01	.2979E-01	.2861E-01	.2676E-01	.2395E-01	.1912E-01	.1196E-01	.2116E-02
16	.2107E-02	.2040E-02	.1838E-02	.1521E-02	.1132E-02	.7172E-03	.3518E-03	.1084E-03	.2411E-04	.2590E-05
20	.9953E-01	.9877E-01	.9654E-01	.9225E-01	.8590E-01	.7603E-01	.6158E-01	.4075E-01	.2044E-01	.4286E-02
23	.3396E-04	.3318E-04	.3079E-04	.2687E-04	.2178E-04	.1579E-04	.9608E-05	.4264E-05	.1452E-05	.1854E-06
30	.4840E-03	.4752E-03	.4485E-03	.4033E-03	.3422E-03	.2651E-03	.1776E-03	.9050E-04	.3545E-04	.5129E-05
35	.4567E-03	.4503E-03	.4308E-03	.3969E-03	.3494E-03	.2857E-03	.2070E-03	.1183E-03	.5248E-04	.9403E-05
48	.4486E-03	.4425E-03	.4238E-03	.3911E-03	.3454E-03	.2836E-03	.2067E-03	.1191E-03	.5326E-04	.9661E-05
50	.1787E-02	.1759E-02	.1674E-02	.1527E-02	.1323E-02	.1054E-02	.7322E-03	.3898E-03	.1583E-03	.2365E-04
51	.2623E-02	.2594E-02	.2508E-02	.2352E-02	.2127E-02	.1803E-02	.1372E-02	.8331E-03	.3906E-03	.7451E-04
56	.3489E-03	.3413E-03	.3180E-03	.2794E-03	.2285E-03	.1673E-03	.1026E-03	.4546E-04	.1514E-04	.1801E-05
64	.9392E-04	.9209E-04	.8667E-04	.7746E-04	.6510E-04	.4975E-04	.3262E-04	.1610E-04	.6104E-05	.8680E-06
66	.9481E-02	.9430E-02	.9276E-02	.8977E-02	.8537E-02	.7823E-02	.6710E-02	.4863E-02	.2604E-02	.4751E-03
109	.3271E-01	.3237E-01	.3130E-01	.2957E-01	.2655E-01	.2253E-01	.1713E-01	.1034E-01	.4788E-02	.9658E-03
125	.3489E-03	.3413E-03	.3180E-03	.2794E-03	.2285E-03	.1673E-03	.1026E-03	.4546E-04	.1514E-04	.1801E-05
143	.3489E-02	.3413E-02	.3180E-02	.2794E-02	.2285E-02	.1673E-02	.1026E-02	.4546E-03	.1514E-03	.1801E-04
144	.3489E-03	.3413E-03	.3180E-03	.2794E-03	.2285E-03	.1673E-03	.1026E-03	.4546E-04	.1514E-04	.1801E-05

Table 3. Species Included in the Updated Model.

Transported Species

1	NITRIC OXIDE	NO
2	NITROGEN DIOXIDE	NO2
3	OZONE	O3
4	HYDROGEN PEROXIDE	H2O2
5	NITRIC ACID	HNO3
6	PAN	PAN
7	NITROUS ACID	HONO
8	NITROGEN PENTOXIDE	N2O5
9	PERNITRIC ACID	HNO4
10	CARBON MONOXIDE	CO
11	>C3 ALKANES	ALKA
12	ETHENE	ETHE
13	TERMINAL ALKENES	PRPE
14	INTERNAL ALKENES	TBUT
15	TOLUENE	TOLU
16	HIGHER AROMATICS	AROM
17	ISOPRENE	ISOP
18	ALPHA-PINENE	PIN
19	FORMALDEHYDE	HCHO
20	ACETALDEHYDE	ALD2
21	METHYL ETHYL KETONE	MEK
22	METHYL GLYOXAL	MGLY
23	GENERAL DICARBONYL	DIAL
24	MATHACROLEIN	MACR
25	METHYL VINYL KETONE	MVK
26	MVK-PAN ANALOG	MPAN
27	HIGHER ALDEHYDE #2	HAC
28	HIGHER ALDEHYDE #3	PCHO
29	PCHO-PAN ANALOG	PIAN
30	ORGANIC PEROXIDE	ROOH
31	O-CRESOL	CRES
32	ALKYL NITRATE	RNO3
33	HYDROPEROXY RADICAL	HO2
34	TOTAL RO2 RADICALS	RO2
35	TOTAL RCO3 RADICALS	RCO3

Steady-State Species

36	OXYGEN- SINGLET D	O*SD
37	HYDROXYL RADICAL	OH
38	ATOMIC OXYGEN	O
39	NITROGEN TRIOXIDE	NO3
40	CRIEGEE BIRADICAL	CRG1
41	CRIEGEE BIRADICAL	CRG2
42	MVK-CRIEGGE RADICAL	MVKO
43	MACR-CRIEGEE #1	MAOO
44	MACR-CRIEGEE #2	MGLO
45	PIN+O3 RADICALS	BIR
46	CH3CO3 RADICAL	MCO3
47	MACR RCO3 RADICAL	MAO3
48	PCHO RCO3 RADICAL	PCO3
49	GENERAL RO2	RO2R
50	GENERAL RO2 #2	R2O2
51	ALKYL NO3 RO2	RO2N
52	PHENOXY RADICAL	BZO

Constant Concentration Species

53	METHANE	CH4
54	WATER VAPOR	H2O

3. THE EMISSIONS INVENTORY

A spatially and temporally resolved inventory of NO_x and hydrocarbon emissions was compiled for a 60 by 81 km region that includes Tampa and St. Petersburg. The NO_x and anthropogenic organics data are inventoried with 3 x 3 km resolution and are based on the Wayne and Kochis (1978) inventory. As shown in Table 4, the anthropogenic NO_x and reactive hydrocarbon emissions are 389 and 381 tons per day, respectively. Figures 1 and 2 illustrate the geographic distribution of anthropogenic emissions. It is important to note that these data are for the year 1976 and that no effort has been made to update the inventory data even though they are clearly out-date. The current anthropogenic emissions inventory may have a significantly different mix of organics, spatial distribution, and HC-to-NO_x ratio so it may not be appropriate to extrapolate the results to current conditions in the study area. Nevertheless, the use of the 1976 inventory is considered acceptable since the purpose of this study is to investigate general relationships between different types of emissions rather than to perform air quality planning for the study area.

The biogenic emission inventory is based on extensive measurements of vegetation emissions made in the study area made by Zimmerman (1979). The reactive biogenic HC emissions in the area are 186 tons per day. The isoprene and monoterpene emissions are 28 and 33 tons per day, respectively. Identification of the remaining portion (ie., 67%) of the biogenic HC emissions is unknown. Based on Zimmerman's approximate classification of the species as alkanes, other alkenes, and aromatics, our inventory includes 33, 64, and 28 tons per day of biogenic alkanes, ethene, and monoalkylbenzenes, respectively. Zimmerman also estimated that there are about 70 tons per day of biogenic methane emissions in the area. The geographic distribution of these emissions are shown in Figure 3. This shows that there are areas with high ($\geq$ 50 μgm/m^2-min) biogenic emission rates fairly close (10-40 km) to the urban centers.

Table 4.

1976 Tampa/St. Petersburg Regional Emissions Inventory.

	Tons Per Day		
Pollutant	Anthropogenic	Biogenic	Total
NO_x	389	0	389
Total Hydrocarbon	230	256	486
Reactive Hydrocarbons	195	186	381
>C3 Alkanes	124	33	157
Ethene	10	64	74
Terminal Alkenes	8	0	8
Internal Alkenes	15	0	15
Mono-alkylbenzenes	18	28	46
Di-/Tri-alkylbenzenes	7	0	7
Isoprene	0	28	28
Mono-terpenes	0	33	33
Formaldehyde	7	0	7
Higher Aldehydes	6	0	6

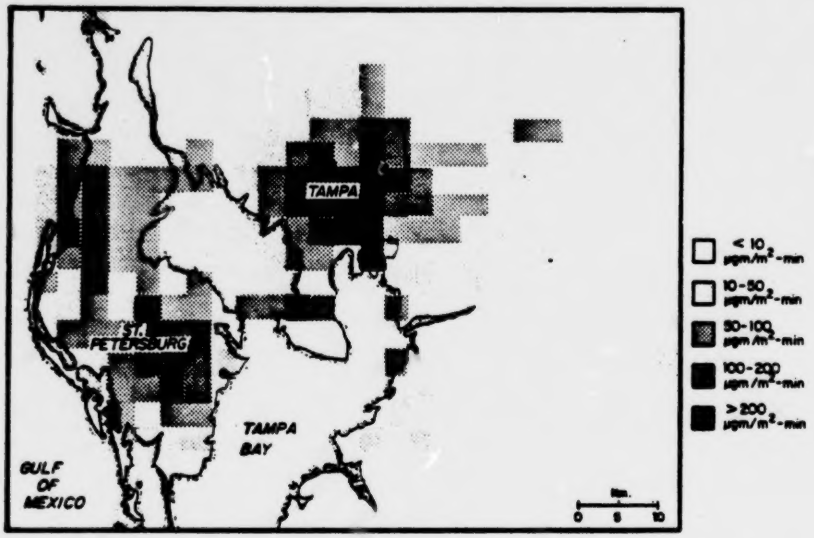
TAMPA
ST. PETERSBURG
TAMPA BAY
GULF OF MEXICO
Km.
0 5 10
< 10 µgm/m²-min
10-50 µgm/m²-min
50-100 µgm/m²-min
100-200 µgm/m²-min
> 200 µgm/m²-min

Fig. 1. Daily average anthropogenic hydrocarbon emission rates (methane included).

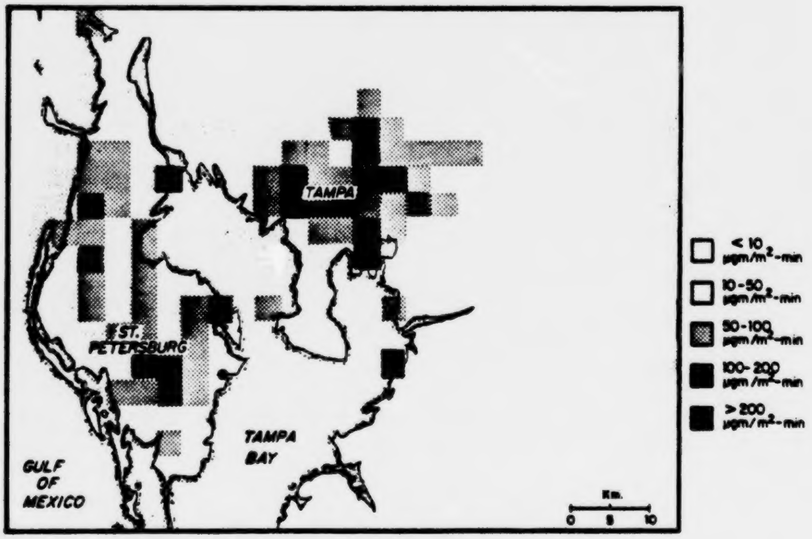
TAMPA
ST. PETERSBURG
TAMPA BAY
GULF OF MEXICO
Km.
0 5 10
< 10 µgm/m²-min
10-50 µgm/m²-min
50-100 µgm/m²-min
100-200 µgm/m²-min
> 200 µgm/m²-min

Fig. 2. Daily average oxides of nitrogen emission rates (as NO_2).

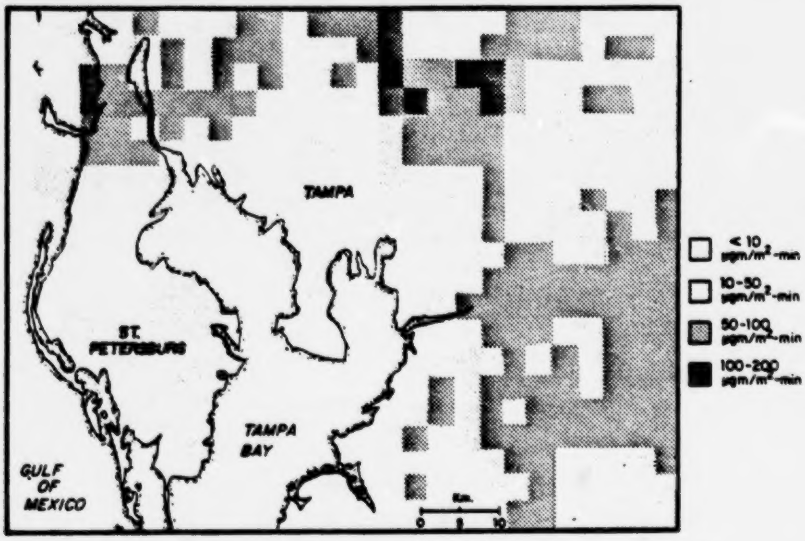
TAMPA
ST. PETERSBURG
TAMPA BAY
GULF OF MEXICO
Km.
0 5 10
< 10 µgm/m²-min
10-50 µgm/m²-min
50-100 µgm/m²-min
100-200 µgm/m²-min

Fig. 3. Daily average biogenic hydrocarbon emission rates (methane included).

4. TRAJECTORY SELECTION

Hourly ozone and surface wind observations were collected at ten and fifteen monitoring stations, respectively, in the Tampa/St. Petersburg area during most of 1977. The three days with the highest network average ozone concentrations were selected for modeling: May 14, June 12, and September 13, 1977. Trajectories that arrived at the monitor locations at the time of maximum daily ozone observations were generated from surface wind data. The trajectories selected for modeling are shown in Figures 4 and 5. These are the identical trajectories used by Lurmann et al. (1984). The trajectory for May 14, trajectory A, shows light northerly winds bring the air parcel into Tampa (the Street Building site, station 25 in Figure 4) at 1430 hour where 105 ppb ozone was observed. The sea breeze strengthens at this hour which advects the parcel to the east and south east. Although this trajectory does not pass the station with the highest ozone on this day, the trajectory is well suited for examining the influence of biogenic HC emissions because it entrained a large amount of biogenic emissions and dispersion conditions were quite limited in the morning hours.

The trajectory for June 12, trajectory B, has moderate strength northerly winds bringing the air parcel into St. Petersburg where 135 ppb of ozone was observed at 1230 hour at the 19th Street - Woodlawn monitor (station 21 in Figure 4). After of an hour of disorganized flow, the sea breeze advects the air parcel fairly rapidly to the east. This trajectory differs significantly from trajectory A in that it entrains less biogenic HC emissions and it has higher initial ozone concentrations (60 ppb in the surface layers). Transported ozone appears to have contributed significantly to the ozone maxima on this day.

The trajectory for September 13 originated in the inland area. The trajectory generated from surface wind data,

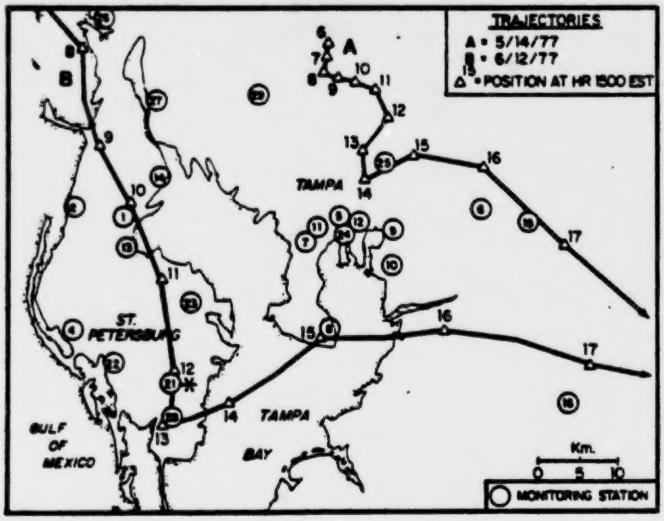
TRAJECTORIES
A = 5/14/77
B = 6/12/77
△15 = POSITION AT HR 1500 EST
A
B
TAMPA
ST. PETERSBURG
TAMPA BAY
GULF OF MEXICO
Km.
0 5 10
○ MONITORING STATION

Fig. 4. Air parcel trajectories for 14 May and 12 June 1977

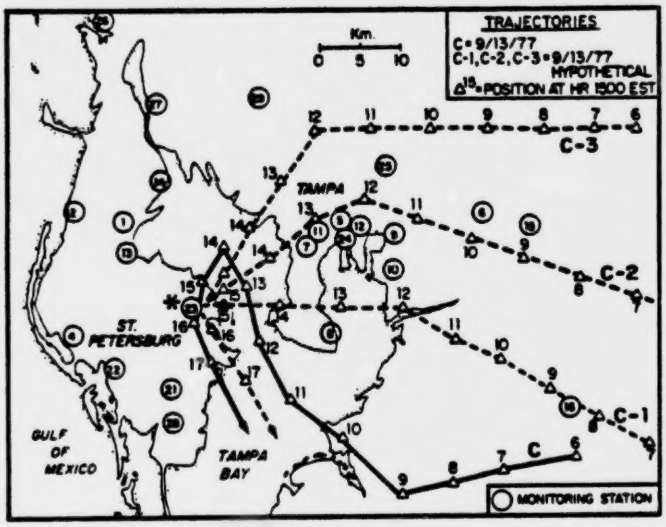
TRAJECTORIES
C = 9/13/77
C-1, C-2, C-3 = 9/13/77 HYPOTHETICAL
△15 = POSITION AT HR 1500 EST
Km.
0 5 10
C-3
C-2
C-1
C
TAMPA
ST. PETERSBURG
TAMPA BAY
GULF OF MEXICO
○ MONITORING STATION

Fig. 5. Air parcel trajectories for 13 September 1977.

trajectory C, begins in the southeastern corner of the modeling domain and it advected by east and southeasterly winds until 1300. Following several hours of disorganized flow, an almost complete flow reversal occurs which brings the air parcel to the 4th Street-Kooger site in St. Petersburg (station 23) where 160 ppb of ozone was observed at 1530 hour. This was the highest ozone observation in the region during 1977. Unfortunately, we have very little confidence in this trajectory because, first, the wind data show onshore flow to both Tampa and St. Petersburg for hours 13 and 14, and, second, very few urban emissions are entrained until the afternoon hours (yet this is the high ozone observation of the year). For these reasons, Lurmann et al. (1984) proposed three additional hypothetical trajectories (C-1, C-2, and C-3) based on the network's daytime average wind speed (~2 m/s). Wind directions for trajectory C-2 were based on the network's average wind direction for 0600-1100, 1200-1500, and 1600-1800 hours. Trajectories C-1 and C-3 were proposed as plausible alternatives. All three hypothetical trajectories entrained more biogenic and anthropogenic emissions than trajectory C (mostly because they spent less time over water).

The average anthropogenic and biogenic emissions rates along each of the trajectories are shown in Table 5. Data are presented for 3 km and 21 km air parcel widths. In the original study, the air parcel width was defined at 3 km in order to take maximum use of the finely resolved emissions inventory. In hind sight, this was probably too narrow and resulted in omissions of some important emission sources. Thus, for the simulations made with the updated model, the emissions were based on a 21 km parcel width. These are calculated by averaging the emissions of seven 3 km wide parallel tracks along the trajectories. The original calculations were made by averaging the emissions along three 1 km tracks parallel to the trajectory. The effects of redefining the parcel width are greater for NO_x than HC emissions. As shown in Table 5, the average NO_x emission rates are substantially higher along trajectories B, C, C-1, and C-2 for the wider parcel. This is primarily a result of entraining emissions from power plants that are missed by the narrow air parcel. With the wider parcel, the hydrocarbon/NO_x ratios of emissions are slightly higher along trajectories A and C-3, slightly lower along trajectory C, and substantially lower along trajectories B, C-1, and C-2. These data also show that 31 to 44% of the HC emissions entrained into the air parcels are from biogenic sources. This is slightly less than is expected based on the regional emissions inventory, where biogenic HCs contribute 49% of the reactive HC emissions. However, this result is consistent with the trajectories since they are oriented towards stations near the center of the urban areas.

Initial species concentrations for the simulations are listed in Table 6. These are identical to those use by Lurmann et al. (1984). Although the region had good coverage with ozone monitors, no upwind NO_x and HC monitors were in operation in 1977. Initial ozone concentrations were assigned values of 10 to 60 ppb below the mixing heights based on the observational data. Above the mixing height, the initial ozone concentration was 80 ppb for all runs. This concentration is probably common aloft at these latitudes in summer. Initial NO_x concentrations of 3 ppb and 40 ppb were used above and below the initial mixing heights, respectively, in all of the simulations. The 40 ppb NO_x is lower than most of the early morning urban observations, yet higher than typical rural values. Initial reactive HC concentrations were set at 100 ppbC and 400 ppbC above and below the initial mixing heights, respectively. Both the initial NO_x and HC concentrations presume the air parcel has been influences by some urban sources (either upwind or by recirculation with the modeling region) and are probably upper limits to the actual concentrations. An additional 5 ppbC of terpenes below the mixing height were included in the runs with biogenic emissions to account for the effects of nighttime emissions.

Table 5.

Average emission rates along the trajectories (in $kg/km^2/hr$).

Traj.	Parcel Width*	Anthropogenic HCs		Biogenic HCs		NO_x	HC/NO_x
A	3	3.6	(64%)**	2.1	(36%)***	3.2	1.8
A	21	2.8	(57%)	2.1	(43%)	2.4	2.0
B	3	2.2	(66%)	1.1	(34%)	1.9	1.7
B	21	1.8	(64%)	1.0	(36%)	3.2	0.9
C	3	1.3	(62%)	0.8	(38%)	1.0	2.1
C	21	1.7	(68%)	0.8	(32%)	1.3	1.9
C-1	3	3.2	(69%)	1.5	(31%)	2.1	2.2
C-1	21	2.4	(64%)	1.3	(36%)	4.4	0.8
C-2	3	1.6	(56%)	1.3	(44%)	0.8	3.7
C-2	21	1.7	(58%)	1.2	(42%)	5.8	0.5
C-3	3	2.8	(68%)	1.3	(32%)	2.6	1.6
C-3	21	3.0	(67%)	1.4	(33%)	2.4	1.8

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* in kilometers.

** Percentage of organics from anthropogenic sources.

*** Percentage of organics from biogenic sources.

Table 6.

Initial Species Concentrations (ppb and ppbC)

Species	Below Mixing Height 14 May	12 June	13 Sept.	Above Mixing Height All Days
Ozone	20	60	10	80
NO	10	5	10	1
NO2	30	35	30	2
Reactive HCs	400	400	400	100
> C3 Alkanes	220	220	220	60
Ethene	60	60	60	15
Propene	12	12	12	1.2
Trans-2-butene	8	8	8	0.8
Toluene	60	60	60	16
Xylenes	20	20	20	2
Formaldehyde	12	12	12	3
Acetaldehyde	8	8	8	1
Terpenes*	5	0	5	0.5
CO	1000	1000	1000	500
CH4**	2000	2000	2000	2000

---

* Included in simulations with biogenic emissions to account for nighttime emissions.

** Included in the updated model simulations.

5. MODEL RESULTS

ELSTAR simulations were performed with the original and updated models for the six trajectories shown in Figures 4 and 5. The baseline calculations were made using the 1976 anthropogenic and biogenic emissions inventory. Additional simulations were performed with 25%, 50%, 75%, and 100% reductions in the anthropogenic HC emissions. Since the initial HC concentrations contribute a significant portion of the total organic loadings, the initial HC concentrations for these simulations were also rolled-back for these simulations. The initial HC concentrations in excess of an assumed 40 ppbC background concentration were reduced by the same percentage that the anthropogenic emissions were reduced. This resulted in initial concentrations of 310, 220, 130, and 40 ppbC below the mixing height and 85, 70, 55, and 40 ppbC above the mixing for the 25%, 50%, 75%, and 100% emission reduction scenarios, respectively. The initial NO_x, ozone, and CO concentrations were not changed for these simulations.

The predicted ozone concentrations from the original model are shown in Figures 6 through 11 for trajectories A through C-3, respectively. The maximum predicted ozone concentrations from each simulation are listed in Table 7. As noted in Lurmann et al. (1984), the original model's baseline simulations underpredict the observed ozone maxima, especially on September 13. This underprediction problem is the reason fairly high initial concentrations of NO_x, HC, and ozone (aloft) were used in the simulations.

The results for the simulations with lower anthropogenic HC emission rates show that initially ozone is formed more slowly than in the baseline simulations. However, the maximum ozone is predicted to be higher than that in the baseline results in 18 of the 24 cases with reduced anthropogenic HC emissions. Even though the magnitudes of the ahthropogenic emission changes are large, the predicted changes in the

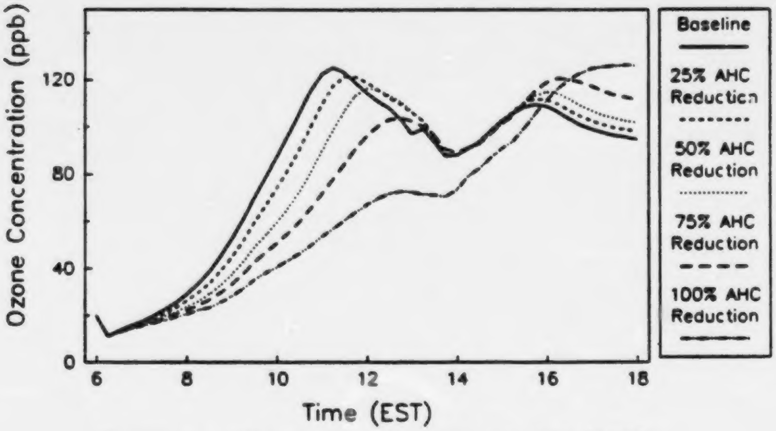

Figure 6. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory A (based on the original model).

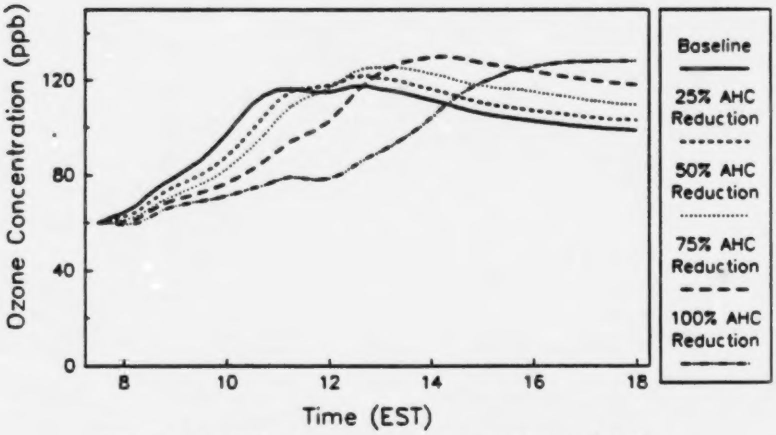

Figure 7. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory B (based on the original model)

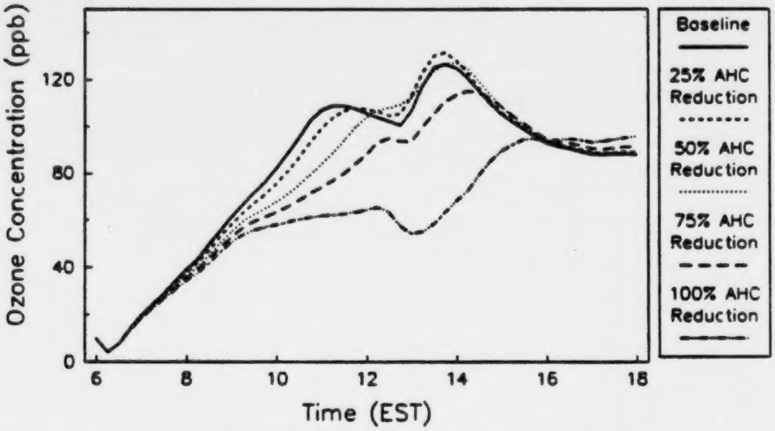

Figure 8. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C (based on the original model).

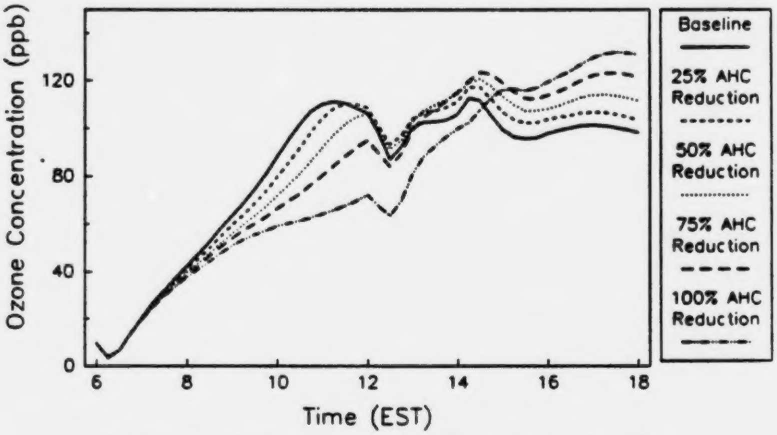

Figure 9. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C-1 (based on the original model).

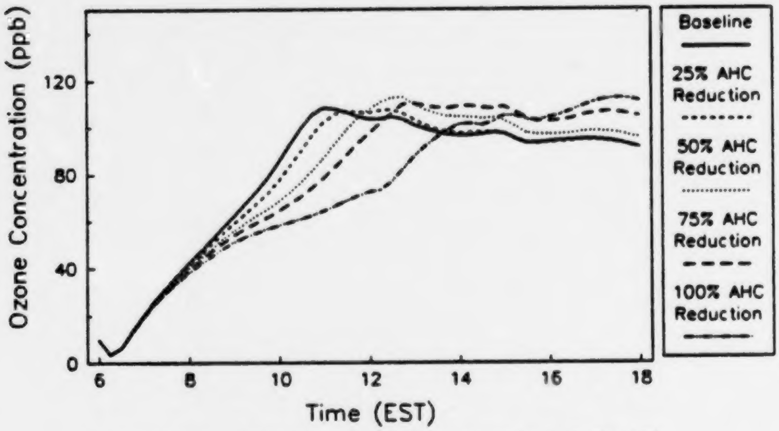

Figure 10. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C-2 (based on the original model).

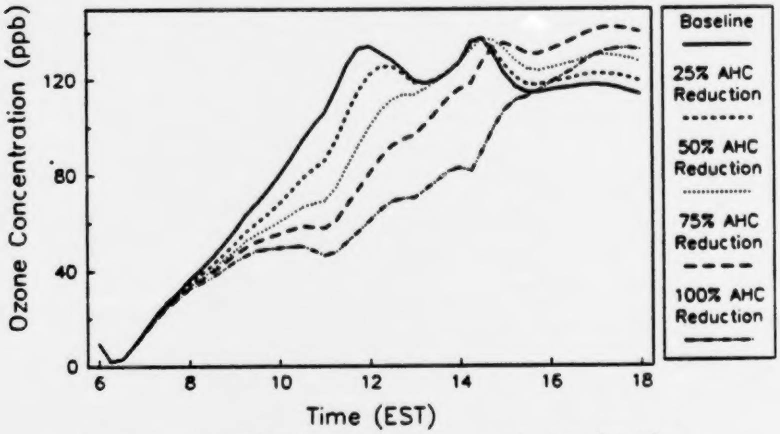

Figure 11. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C-3 (based on the original model).

Table 7.

Maximum ozone concentrations (ppb) predicted by the original model.

Traj.	Baseline	25% AHC Reduction	50% AHC Reduction	75% AHC Reduction	100% AHC Reduction
A	125	122	116	121	126
B	118	122	126	130	128
C	127	132	127	115	96
C-1	113	117	121	124	132
C-2	108	108	113	111	113
C-3	134	138	138	142	133

Table 8.

Percentage change in the maximum ozone concentrations predicted by the original model.

Trajectory	25% AHC Reduction	50% AHC Reduction	75% AHC Reduction	100% AHC Reduction
A	-2	-7	-3	0
B	+3	+7	+10	+8
C	+4	0	-9	-24
C-1	+3	+7	+10	+17
C-2	0	+5	+3	+5
C-3	+3	+3	+6	-1

maximum ozone are small (see Table 8). For example, with 25% reduction in anthropogenic HCs the change in maximum ozone range from -2% to +4% and with 75% reduction in anthropogenic HCs the change in maximum ozone ranged from -3% to +10%. It is important to note that the ozone maxima associated with the reduced anthropogenic HCs occur later in the day than those in the baseline simulations, especially for the case with 100% AHC reduction. These results suggest that anthropogenic HC emission reductions might be effective for reducing concentrations at urban and suburban locations passed in midday, however, farther downwind they are not predicted to be effective in most cases. This suggests the biogenic emissions contribute sufficient reactivity that even in the absence of the anthropogenic HC emissions, ozone can be formed fairly rapidly from the urban NO_x emissions and, in some case, in greater amounts than when the anthropogenic emissions are present. This latter result should be viewed very cautiously because it is not consistent with the results from the updated model which employs a more accurate chemical mechanism.

The updated model's ozone prediction for the baseline cases and the anthropogenic HC reduction scenarios are shown in Figures 12, 14, 16, 18, 20, and 22. Comparisons of the baseline results with the scenario of 100% biogenic HCs reduction are shown in Figures 13, 15, 17, 19, 21, and 23. Table 9 shows the predicted maximum concentrations for these runs and Table 10 lists the changes in maximum ozone concentrations from the baseline run for all scenarios. The updated model's baseline results exceed the observed ozone maxima for trajectories A and B, and underestimate the observed maxima trajectories C, C-1, C-2, and C-3. The differences in the baseline predictions between the original and updated models are due to both differences in the chemical mechanism and the emissions. The calculations for the 100% biogenic HC reduction scenario made with the updated model show 2 to 11% reduction in the maximum ozone which is entirely consistent

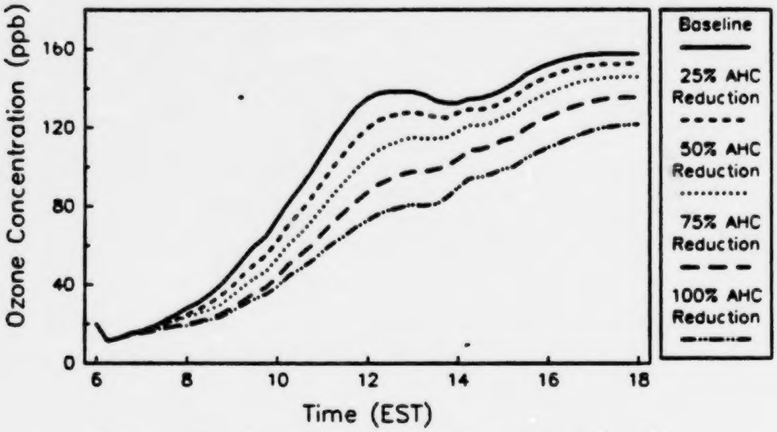

Figure 12. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory A (based on the updated model).

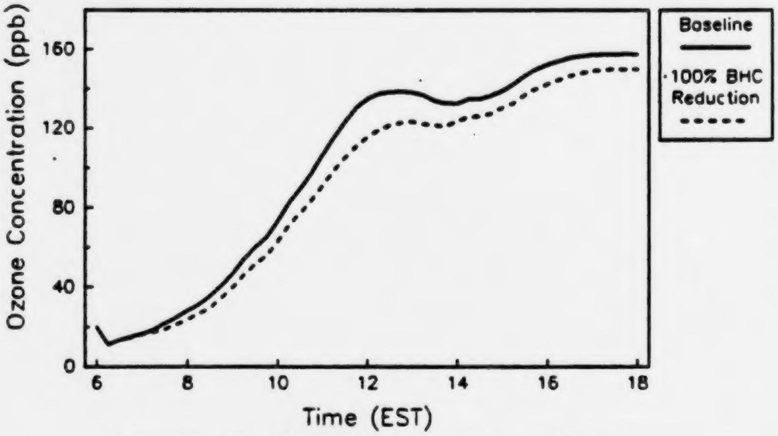

Figure 13. Effects of biogenic HC (BHC) reductions on predicted ozone along Trajectory A (based on the updated model).

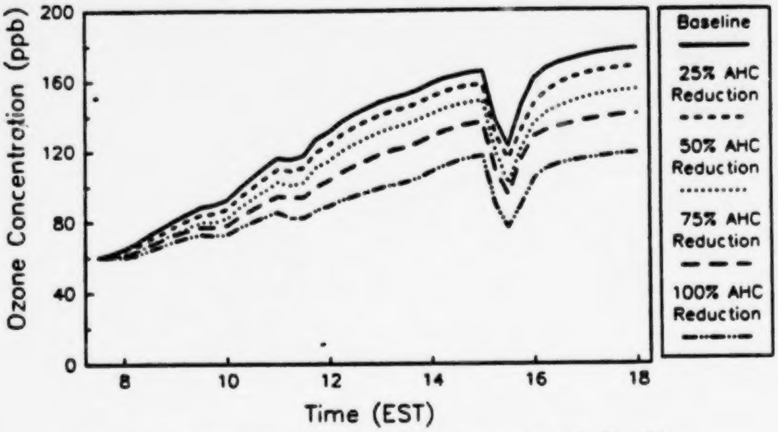

Figure 14. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory B (based on the updated model).

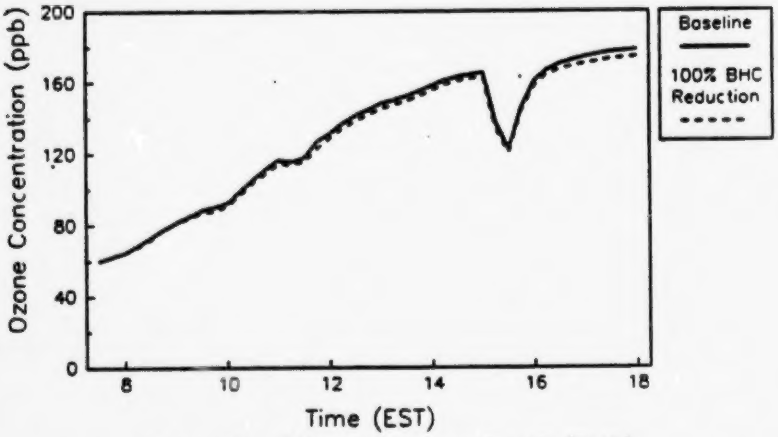

Figure 15. Effects of biogenic HC (BHC) reductions on predicted ozone along Trajectory B (based on the updated model).

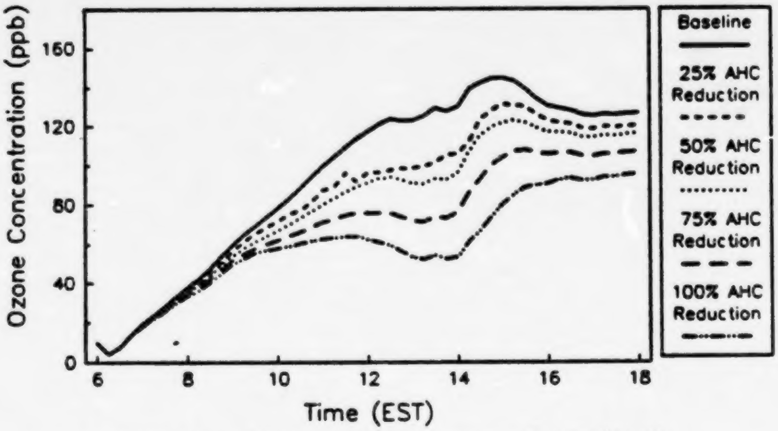

Figure 16. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C (based on the updated model).

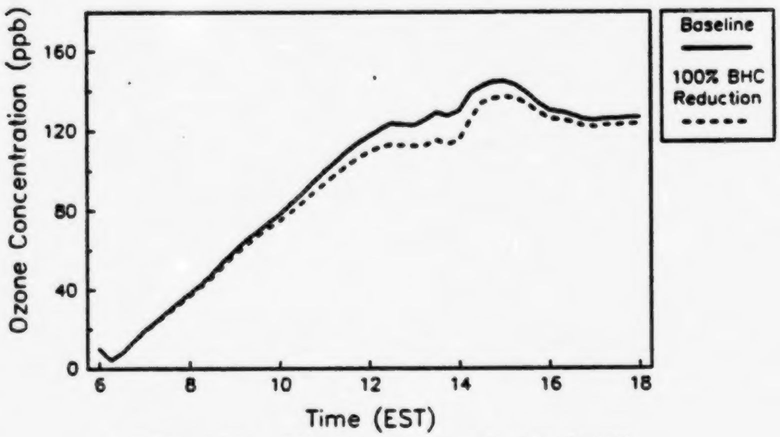

Figure 17. Effects of biogenic HC (BHC) reductions on predicted ozone along Trajectory C (based on the updated model).

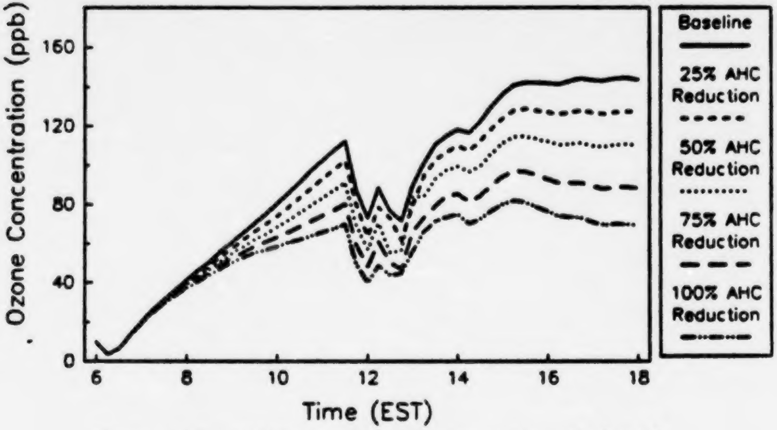

Figure 18. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C-1 (based on the updated model).

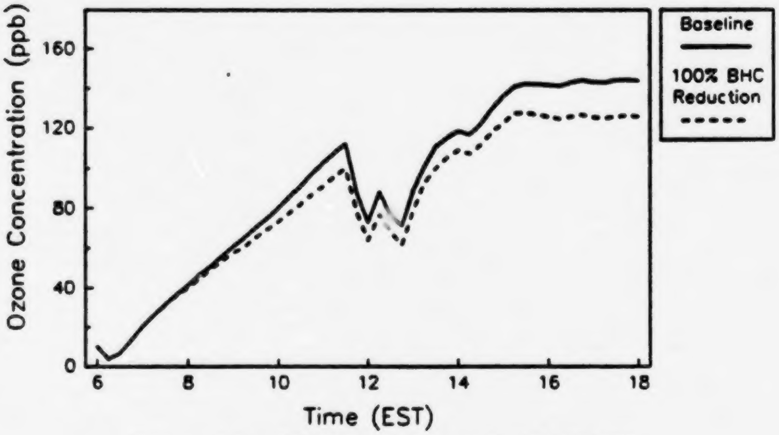

Figure 19. Effects of biogenic HC (BHC) reductions on predicted ozone along Trajectory C-1 (based on the updated model).

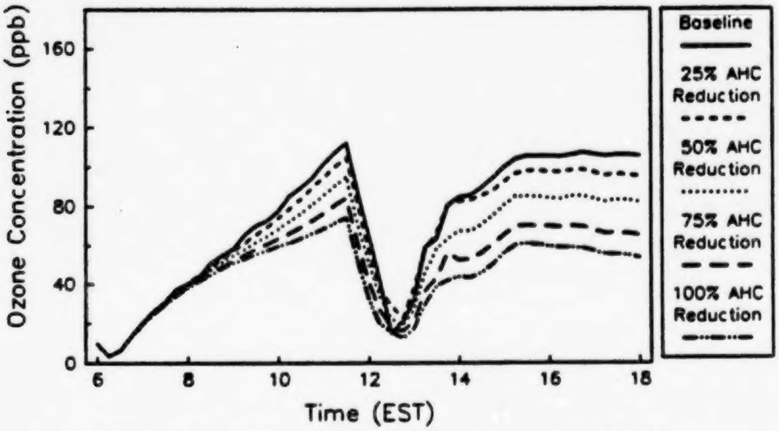

Figure 20. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C−2 (based on the updated model).

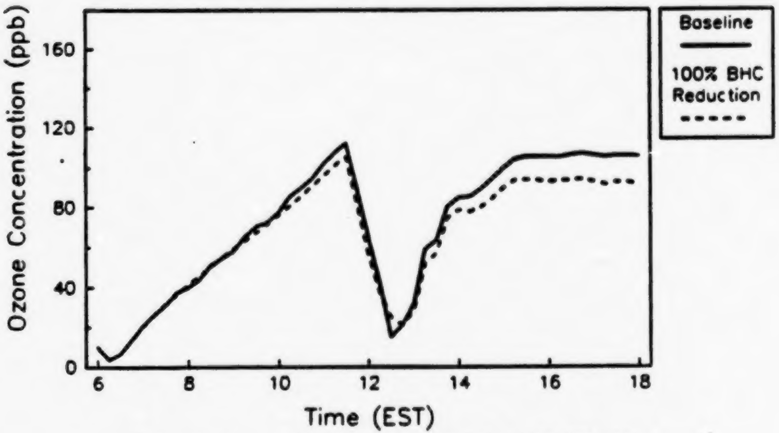

Figure 21. Effects of biogenic HC (BHC) reductions on predicted ozone along Trajectory C−2 (based on the updated model).

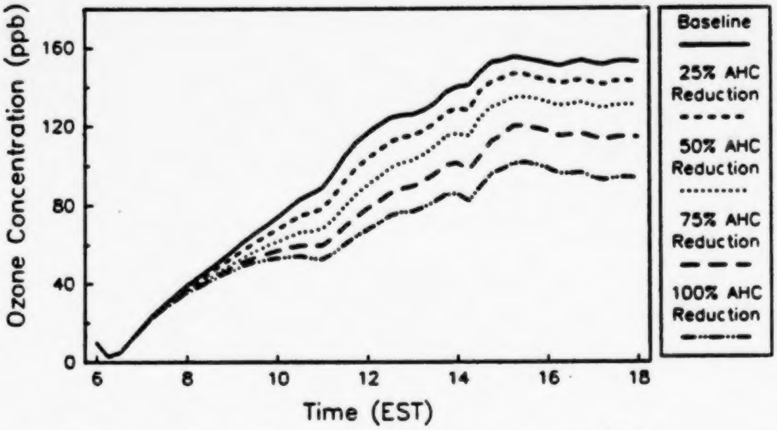

Figure 22. Effects of anthropogenic HC (AHC) reductions on predicted ozone along Trajectory C-3 (based on the updated model).

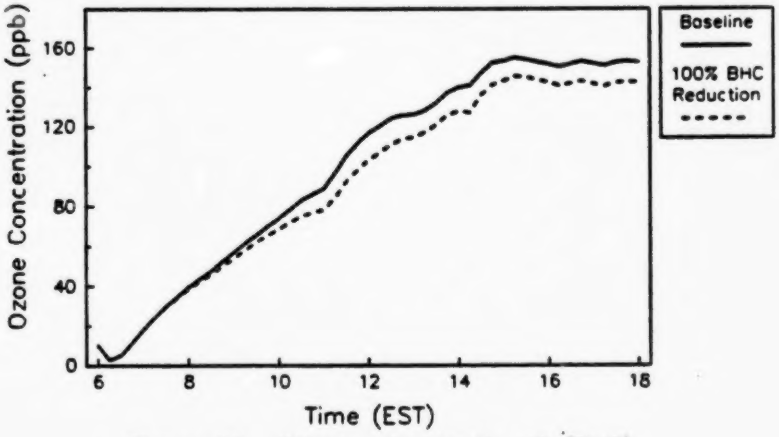

Figure 23. Effects of biogenic HC (BHC) reductions on predicted ozone along Trajectory C-3 (based on the updated model).

Table 9.

Maximum ozone concentrations (ppb) predicted by the updated model.

		Emission Reduction Scenario				
Traj.	Baseline	25% AHC	50% AHC	75% AHC	100% AHC	100% BHC
A	158	153	146	136	122	150
B	178	168	155	141	119	174
C	145	131	123	108	96	137
C-1	144	129	115	97	82	128
C-2	112	105	95	85	75	105
C-3	155	147	135	120	102	146

Table 10.

Percentage change in the maximum ozone concentrations predicted by the updated model.

Traj.	25% AHC Reduction	50% AHC Reduction	75% AHC Reduction	100% AHC Reduction	100% BHC Reduction
A	-3	-8	-14	-23	-5
B	-6	-13	-21	-33	-2
C	-10	-15	-26	-34	-6
C-1	-10	-20	-33	-43	-11
C-2	-6	-15	-24	-33	-6
C-3	-5	-13	-23	-34	-6

with the 2% to 9% reported in the earlier study.

All of the updated model simulations with reduced anthropogenic HC emissions show slower ozone formation rates and lower maximum ozone concentrations than the baseline runs. Also, for all cases, the magnitudes of the changes in maximum ozone are consistent with the magnitudes of the anthropogenic HC reductions. That is, progressively larger emission reductions are predicted to result in progressively lower ozone concentrations (which is not the case with the original model's results). The range of effectiveness of anthropogenic HC controls along these trajectories are as follow:

> with 25% reduction, maximum ozone concentrations are predicted to decrease by 3 to 10%;

> with 50% reduction, maximum ozone concentrations are predicted to decrease by 8% to 20%;

> with 75% reduction, maximum ozone concentrations are predicted to decrease by 14% to 33%; and

> with 100% reduction, maximum ozone concentrations are predicted to decrease by 23% to 43%.

Since the background ozone levels are fairly high in these simulation (approximately 70 ppb for the column average), it also is worthwhile to look at the effects of these reduction on the "controllable" portion of the ozone (ie., the portion that exceeds the initial or background ozone). Table 11 shows the percentage changes in the portion of the ozone that exceeds the a 70 ppb background. The predicted reductions in the "controllable" ozone are 2 to 2.5 times larger than the reductions in total ozone. For example, the 50% and 100% reductions in anthropogenic HCs are predicted to reduce the "controllable" ozone by 14% to 40% and 41% to 88%, respectively. These clearly show that anthropogenic HC reductions can be effective in some cases.

The difference in the effectiveness of anthropogenic HC reduction is largely explained by the NO_x and biogenic HC

Table 11.

Percentage change in the maximum ozone exceeding the 70 ppb background, from the updated model.

Traj.	25% AHC Reduction	50% AHC Reduction	75% AHC Reduction	100% AHC Reduction	100% BHC Reduction
A	-6	-14	-25	-41	-9
B	-9	-21	-34	-55	-4
C	-19	-29	-49	-65	-11
C-1	-20	-39	-64	-84	-22
C-2	-16	-40	-64	-88	-17
C-3	-9	-23	-41	-62	-11

emission rates on different trajectories. Trajectory A has the highest biogenic emission rate and the second lowest NO_x emission rate. The results for trajectory A are typical of a photochemical system operating in the high HC/NO_x regime, where hydrocarbon reductions have only a small effect on the maximum ozone because there is essentially an excess of organics in the system (even after controls). In contrast, trajectories C-1 and C-2, which have moderate biogenic emission rates and the highest NO_x emission rates, respond like photochemical systems operating in the lower HC/NO_x regime where HC reductions are known to be effective. The other three cases have emission rates that place them between these two extremes and their response to the HC emission reductions is also in between the two extremes.

Additional simulations have been performed to examine the effects of ignoring biogenic HCs in control strategy calculations. Simulations of trajectory A with 25%, 50%, and 75% anthropogenic HC reductions were performed without biogenic emissions. Figure 24 compares the predicted ozone in these runs with those for a run with 100% of the anthropogenic emissions and without biogenic HCs. The effects of the 25%, 50%, and 75% anthropogenic HC reductions are to reduce the maximum ozone from 150 ppb to 144, 132, and 117 ppb, respectively. The predicted ozone reductions of 4%, 12%, and 22% for the three scenarios are only slightly larger than the 3%, 8%, and 14% reductions calculated with biogenic emissions included. However, if these results were used for a control strategy calculation for a day with a 150 ppb design value, the AHC control requirement would be 70% if the biogenic HCs were ignored and 92% if they were included. Since urban AHC emission reductions as large as 70% may be achievable, yet reductions greater than 90% are almost certainly not achievable with known technologies, policy-makers would probably make different choices on which pollutants to control given these two sets of results. These results clearly confirm that

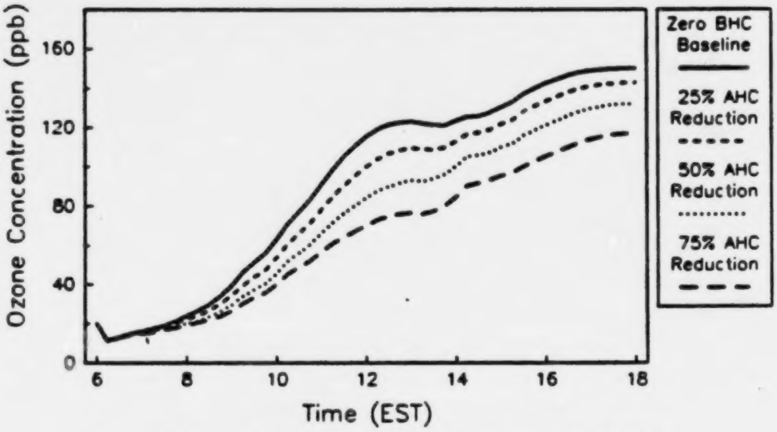

Figure 24. Effects of anthropogenic HC (AHC) reductions with biogenic HCs ignored along Trajectory A (based on the updated model).

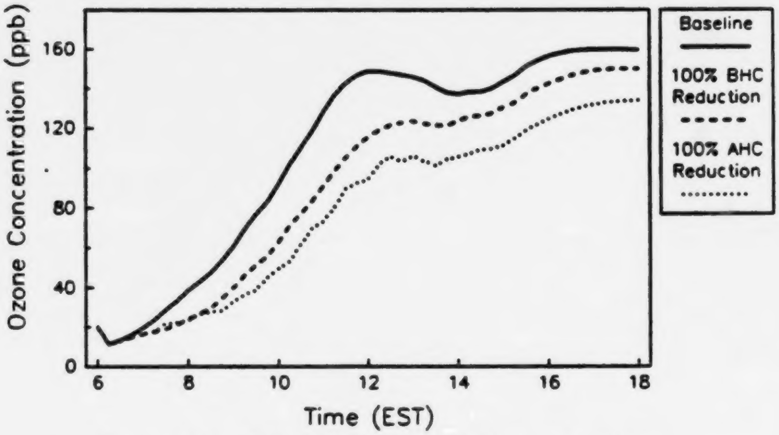

Figure 25. Effects of HC emission reductions with all biogenics as treated isoprene along Trajecory A (based on updated model).

omitting the biogenic HC can lead to underestimation of the HC control requirement needed to meet the standard in cases with high biogenic emissions rates. However, the amount of the underestimation for the Tampa/St. Petersburg trajectory with the highest biogenic emissions rate is substantially smaller (22%) than reported by Chameides et al. (1988) for Atlanta (70%) for comparable design values. The difference is partially be explained by the fact that the highest daily average biogenic emissions rate in this study is only half as large as that used by Chameides et al. and, as discussed below, the Tampa/St. Petersburg biogenic emissions is less reactive than that assumed for Atlanta. Nevertheless, our results suggest that in order to develop effective and reliable ozone strategies, the biogenic emissions should be included in the emission inventories for regions where these emissions could be high (ie., heavily vegetated areas).

One difference between the biogenic emissions inventory for Tampa/St. Petersburg and those employed in other studies is that there is a smaller amount of isoprene (probably the most reactive biogenic species) in the Tampa/St. Petersburg inventory. Also, our assignments of the 67% unidentified biogenic HCs to HC classes may underestimate the reactivity of these species. In order to investigate the influence of this characteristic (and assumptions), simulations were made assuming all biogenic emissions along trajectory A were isoprene. Figure 25 shows the results for a baseline case and a case with 100% anthropogenic HC reduction with all biogenics treated as isoprene. It also show the 100% biogenic HC reduction results. In the baseline simulation, ozone is formed slightly more rapidly when all biogenics are treated as isoprene (see Figures 12 and 13 for comparison), however, the maximum ozone is only 2 ppb higher at the end of the run (the time of the maximum in both runs). The amount of ozone formed when anthropogenic HCs are reduced by 100% is significantly greater when the biogenic emissions are treated as isoprene.

The maximum ozone is reduced by only 16%, instead of 23%. These results are consistent with the recognized high reactivity of isoprene and general characteristic of photochemical systems operating in the high HC/NO_x regime. The effects would almost certainly be greater for runs with lower HC/NO_x ratios. These results illustrate the need for studies to carefully identify the biogenic species and to determine their reactivity and chemical reaction mechanisms. Such studies are needed to accurately quantify the biogenic HC's influence on ozone.

Lastly, several simulations were performed to examine the effects of reducing NO_x emissions instead of anthropogenic HC emissions. Simulations of trajectory A with 25%, 50%, and 75% reductions in NO_x emissions (and initial NO_x concentrations) were performed. The results, shown in Figure 26, indicate that ozone initially increases more rapidly, however, the maximum ozone is reduced from the baseline result of 158 ppb to 145, 127, and 102 ppb with the 25%, 50%, and 75% reductions in NO_x, respectively. This indicates that 25% and 50% reductions in NO_x are comparable to 50% and 90% reductions in anthropogenic HC, respectively, in terms of reducing maximum ozone concentrations on this trajectory. While the effects of NO_x reductions probably would not be as large (and maybe counter productive) on the other trajectories that have lower biogenic HC emissions and higher NO_x emissions, this case does illustrate that ozone reductions may be achieved with smaller percentage reductions in NO_x emissions than in anthropogenic HC emissions in some cases.

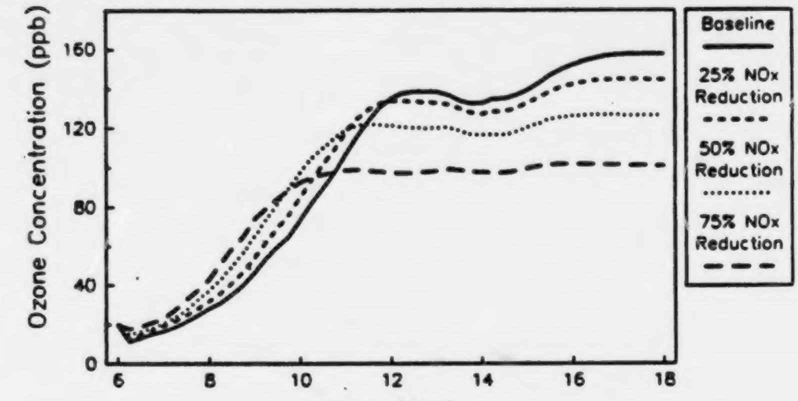

Figure 26. Effects of NOx emission reductions on ozone along Trajectory A (based on the updated model).

6. CONCLUSIONS

An assessment of the effects of anthropogenic HC emission reductions has been made for Tampa/St. Petersburg, an urban area with high biogenic HC emission. The results of the assessment should be interpreted cautiously since the emission rates and atmospheric chemical reactions of the biogenic HCs are highly uncertain. ELSTAR photochemical trajectory model simulations were performed with a chemical mechanism used in the 1984 Lurmann et al. study and an updated chemical mechanism. The results with the 1984 chemical mechanism produced some inconsistent results and are not considered as reliable as the results calculated with the updated mechanism.

The results with the updated mechanism indicate that the effects of anthropogenic HC reductions on maximum ozone
centrations depend on the rates of biogenic and NOx
ssions. For the case with the highest biogenic emissions
e and second to the lowest NOx emissions rate (trajectory A), 25%, 50%, 75% and 100% reductions in anthropogenic HCs were predicted to reduce the maximum ozone by 3%, 8%, 14%, and 23%, respectively. For a case with lower biogenic emission rates and higher NOx emission rates (trajectory C-1), 25%, 50%, 75%, and 100% reductions in anthropogenic HCs were predicted to reduce the ozone by 10%, 20%, 33%, and 43%, respectively. A relative high ozone background concentrations was used for all of the calculations so it is unlikely that any amount of emission reductions could produce more than about a 60% reduction in the ozone is these case. Ozone was formed more slowly in all of the simulations with reduced anthropogenic HCs, however, in some of the simulations there was sufficient reactivity contributed by biogenic emissions to produce almost as much ozone (ie., up to 77% of the baseline run concentration) without the anthropogenic HCs as with them. In other case with higher NOx emissions, anthropogenic HC

reductions appeared to be more effective.

Simulations were performed to examine the effects of ignoring biogenic HCs in control strategy calculations for the trajectory with the highest biogenic emissions rate. When the biogenics were excluded, ozone reductions of 4%, 12%, and 22% were calculated for anthropogenic HC reductions of 25%, 50%, and 75%, which are only slightly larger than the 3%, 8%, and 14% reductions calculated with biogenic emissions included, respectively. However, if these results are used for a control strategy calculation for a day with a 150 ppb design value, the AHC control requirement would be 70% if the biogenic HCs were ignored and 92% if they were included. Since urban AHC emission reductions as large as 70% may be achievable, yet reductions greater than 90% are almost certainly not achievable with known technologies, policy-makers would probably make different choices on which pollutants to control given these two sets of results. These results clearly show that omitting the biogenic HC can lead to underestimation of the HC control requirement needed to meet the standard in cases with high biogenic emissions rates. However, the amount of the underestimation for the Tampa/St. Petersburg trajectory with the highest biogenic emissions rate was substantially smaller (22%) than reported by Chameides et al. (1988) for Atlanta (70%) for comparable design values. The difference may partially be explained by the fact that the emission rates and reactivity of the biogenic species in the Tampa/St.Petersburg simulations were lower than those assumed by Chameides et al.. Nevertheless, the Tampa/St. Petersburg results suggest that in order to develop effective and reliable ozone strategies, the biogenic emissions should be included in the emission inventories in regions where these emissions could be high (ie., areas heavily vegetated with plant species known to emit reactive hydrocarbons).

Analyses were carried out to examine the sensitivity of the results to the composition of the biogenic emissions.

Simulations with all of the biogenic HC emissions treated as isoprene showed smaller reductions in ozone when anthropogenic HCs were reduced. This illustrates the need for better identification of the biogenic species and better chemical mechanisms for these species (as well as the obvious need for reliable emissions data).

A limited number of simulations were performed to examine the effects of NO_x emission reductions. For the case with the highest biogenic emissions rate, 25%, 50%, and 75% reductions in NOx emissions produced larger reductions in ozone than were produced by the same percentage reductions in anthropogenic HC emissions. Or interpreting the results another way, 25% and 50% reductions in NO_x could be as effective in reducing maximum ozone as 50% and 90% reductions in anthropogenic HC, respectively, on one trajectory. While the effects of NO_x reductions probably would not be as large (and maybe counter productive) on the other trajectories that have lower biogenic HC emissions and higher NO_x emissions, this case does illustrate that ozone reductions may be achieved with smaller percentage reductions in NO_x emissions than anthropogenic HC emissions in some cases.

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APPENDIX B

SENSITIVITY OF EKMA MODEL PREDICTIONS TO BIOGENIC EMISSIONS

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SECTION 1

INTRODUCTION

In a recent article published in Science, the role of biogenic organic emissions in urban ozone formation was examined (Chameides, et al., 1988). The article described a study in which the Empirical Kinetic Modeling Approach (EKMA) was applied to the metropolitan Atlanta region. EKMA model simulations were conducted with and without biogenic emissions to assess their effect on ozone production under existing conditions and to evaluate their impact on estimated reductions in emissions of ozone precursors that may be needed to achieve the National Ambient Air Quality Standard (NAAQS) for ozone. An important outcome of that study is that including biogenic emissions in model simulations of existing conditions does not substantially alter predictions of peak ozone, but it significantly increases the estimated reduction in emissions of volatile organic compounds (VOC) from anthropogenic sources that would be needed to attain the ozone NAAQS. As a result, the authors conclude that it is essential to account for the effect of biogenic emissions in the development of control strategies for attaining the ozone NAAQS. EPA guidelines for applying EKMA do not currently contain provisions for including the effects biogenic emissions (EPA, 1987).

The modeling study described by Chameides et al. consisted of applying the EKMA model to a single ozone episode in the Atlanta region using a fixed set of assumptions regarding the emissions of biogenic organics. The purpose of this paper is to describe a series of analyses conducted with the same model to examine the sensitivity of these findings to other conditions and assumptions. The tests conducted as part of this effort were primarily directed towards determining the sensitivity of model predicted control estimates for both VOC and nitrogen oxides (NO_x) to the inclusion of biogenic emissions. They were designed to provide information on the following general areas of concern with respect to EKMA applications:

1) the impact of including biogenic emissions on VOC and NO_x control estimates for the Atlanta area;
2) the effect of using different spatially and temporally resolved biogenic emission inventories;
3) the effect of biogenic VOC speciation;
4) the effect of delayed interaction of urban plumes with rural areas (e.g., larger versus smaller urban areas and/or slower versus higher wind speeds); and,
5) the potential impact of biogenic VOC emissions in other areas of the country;

To carry out these tests, the data base and assumptions described by Chameides et al. were used, as well as other sources of information on anthropogenic and biogenic emissions for Atlanta and other areas of the country.

As noted above, the sensitivity tests described in this paper were performed using the EKMA model. EKMA has been widely used in the past in the development of control strategies to reduce ambient ozone concentrations, and several guidance documents have been developed by EPA for that purpose (U.S. EPA, 1977; U.S. EPA, 1981; U.S. EPA, 1984; U.S. EPA, 1987). The particular version of EKMA used in this study is the one incorporating the Carbon Bond IV chemical mechanism (CB-4) in the OZIPM4 computer program (Gery et al., 1988;

Hogo and Gery, 1988; and U.S. EPA, 1987). This is the same model that was used by Chameides et al. in their study, although some minor modifications have been made to the computer programs. A complete description of this version of EKMA is contained in the previously cited references, so no further discussion of the model itself is included here. Appendix A contains a brief description of how the CB-4/OZIPM4 model was used in conducting the analyses described in the ensuing sections.

Before proceeding with the description of the tests conducted as part of this study, two subjects warrant further discussion. First, in this study EKMA has been used to estimate reductions in emissions of ozone precursors that may be needed to lower ozone concentrations to the level of the ozone NAAQS. Throughout this report, these emission reductions will be referred to as control estimates. They are not meant to imply the actual degree of control that would be required to attain the ozone NAAQS in any particular nonattainment area however. To determine nonattainment control targets, EPA guidelines recommend that a number of ozone episodes occurring in the nonattainment area be modeled (U.S. EPA, 1987). The control target for attaining the NAAQS is then selected from those results according to the statistical form of the ozone standard (i.e., the degree of control that insures that there is no more than one exceedence of 0.12 ppm per year, on average, at each monitoring site). Since a limited number of episodes are considered in this study, it is only possible to provide information on the relative change in control estimates that may occur when biogenic emissions are considered. Second, differences in estimates of both biogenic and anthropogenic emissions are found with the various sources of information used in this study. Although these differences are described, any attempt to reconcile them is beyond the scope of this study. Instead, this effort is limited to identifying those differences and to determining the effects they have on model predictions.

The remainder of this paper is divided into four sections. Section 2 describes a series of initial modeling analyses performed using the same basic assumptions of Chameides et al. and some additional simulations that were conducted to test the sensitivity of these results to variations in other model inputs. Section 3 describes the results of additional EKMA modeling of the Atlanta region using different data bases for both biogenic and anthropogenic emissions. Section 4 contains an assessment of whether the findings for the Atlanta region are universally applicable to other areas of the country as well. The final section summarizes the major findings and conclusions arising from the analyses described in the three previous sections.

SECTION 2

INITIAL ANALYSES

This section describes the results of sensitivity tests conducted with the EKMA model using essentially the same assumptions as those used in the study reported by Chameides et al. The starting point for these analyses involved replicating, to the extent possible, the model simulations described in the Science article in order to insure that no confounding effects are introduced by major differences in the computer program or chemical mechanism used in this study. Additional tests were then conducted to examine the sensitivity of those results to the magnitude and timing of biogenic emissions, to evaluate other episodes in Atlanta, and to test the sensitivity to changes in other EKMA inputs such as the VOC/NO_x ratio, dilution, post-0800 anthropogenic emission rates, and the reactivity of anthropogenic emissions. In the discussions that follow, both VOC and NO_x control estimates are reported. These control estimates have been calculated assuming that no change occurs in the emissions of the other precursor. For example, a 40% VOC control estimate implies that, in order to lower peak ozone to 0.12 ppm, emissions of VOC must be reduced by 40% with no concurrent change in NO_x emissions. Also, as reported in this paper control estimates always refer to reductions of anthropogenic emissions only (i.e., potential changes in biogenic emissions are not considered).

MODEL REPLICATIONS

The analysis described in the Science article by Chameides et al. involved applying the EKMA model to simulate conditions associated with a single exceedence of the ozone NAAQS measured on June 4, 1984 at a monitoring site located to the southeast of Atlanta at Conyers, Georgia. Except for the inclusion of biogenic emissions, the model inputs used in the EKMA simulations were derived from data used by the Georgia Department of Natural Resources (GDNR) in the development of the 1987 State Implementation Plan (SIP) for Atlanta. An example set of EKMA model inputs with biogenic emissions and the corresponding output generated by the model were supplied by Chameides, and are shown in Appendix B (Chameides, 1989). Appendix B also contains model output generated as part of this effort for the same example. The two outputs are virtually identical, with the small differences that do occur attributable to computer differences. These results demonstrate that no significant differences exist between the model used by Chameides et al. and the one used for this study.

Although the example simulation supplied by Chameides was successfully reproduced as part of this study, it does not include any calculations of control estimates. As reported in the Science article, the VOC control estimate for the exceedence that was modeled increased from 30% to 70% when a 30 kg/km^2/day emission rate of isoprene was included in the simulations. In an attempt to reproduce these results, the model inputs shown in Appendix B were used with OZIPM4/CB-4 to perform control calculations for these two cases. For the case with no isoprene emissions, the VOC control estimate was found to be 31%, virtually identical to that reported in the Science article. Some ambiguity does exist, however, with respect to the other case. The isopleth diagrams shown in the Science article suggest that the VOC control estimate for the case with isoprene emissions may have been calculated using the model predicted peak ozone (versus the observed peak) as the ozone design value (i.e, the starting point for the control calculations). When the predicted peak is used as the design value, the calculated VOC control estimate found for this study is nearly the same as that reported in the journal article, 72% compared to 70%. A slightly higher estimate, 77%, is found when the observed peak is used. Regardless of which design value is used, however, the effect is the same: the VOC control estimate is substantially higher when isoprene emissions of this magnitude are included in the model simulations. Thus, even though the calculated control estimates differ slightly, the modeling results produced as part of this effort are in substantial agreement with the those reported by Chameides et al.

Aside from the inclusion of isoprene emissions, the example simulation shown in Appendix B deviates somewhat from recommended procedures for applying EKMA (U.S. EPA, 1987). To make the sensitivity tests that are described below more compatible with the current EPA guidelines, the following changes were made: the simulation was started at 0800 Local Daylight Time (LDT), the simulation length was reduced to 11 hours, the input time zone was changed from 5 to 4, and the anthropogenic emissions for the last two hours altered based on supplemental information contained in the SIP (Baugues, 1989). (Although current guidelines recommend a simulation length of ten hours, eleven hours was used here because the VOC control estimates are slightly higher for the longer periods. Longer simulation periods do not significantly affect control estimates for this case.) With these changes, the VOC control estimates obtained using the observed ozone concentration as the design value are 86 and 31 percent with and without isoprene emissions, respectively. The increase from 77% to 86% in the VOC control estimate for the case with the biogenics is primarily due to the change in the time zone input variable. Note that these changes do not in any way lessen the impact of the biogenic emissions. The revised model inputs are listed in Appendix C, and are used as the basis for most of the sensitivity tests discussed below.

SENSITIVITY TO ISOPRENE EMISSIONS

As described in their article, Chameides et al. estimated that, during the summer in Atlanta, the total biogenic VOC emission rate averaged across the region is approximately 50 kg/km^2 for a 15 hour daylight period. Of the total biogenic VOC emitted, they estimate that about 30 kg/km^2 is isoprene. In their modeling analysis, all biogenic emissions were represented as isoprene (ISOP) in the CB-4 mechanism. In this subsection, the sensitivity of the EKMA model predictions to the magnitude and timing of isoprene emissions is examined. In these tests, the EKMA model inputs listed in Appendix C are used, and the same diurnal distribution of isoprene emissions that was used by Chameides et al. is employed. With this distribution, emissions are zero at 0800 LDT, increase linearly until 1200 LDT, remain constant for three hours, and then decrease linearly to zero at 1900 LDT. Figure 1 shows the fraction of the total isoprene emitted during the simulation that is emitted each hour. No isoprene is assumed to be present at the beginning of the simulation.

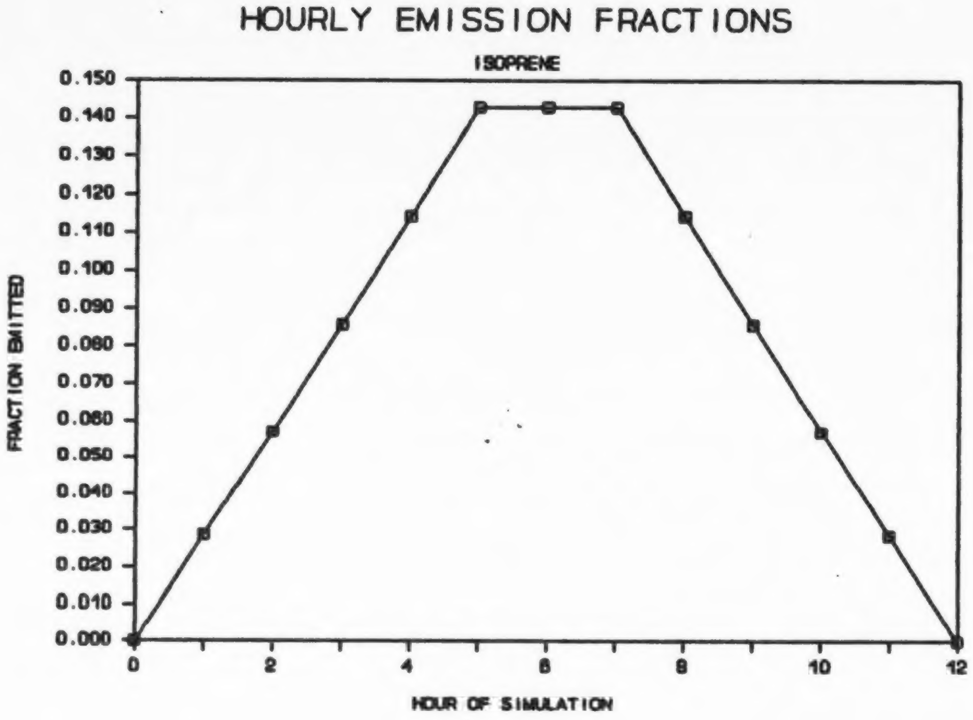


Figure 1. Diurnal Distribution of Isoprene Emissions used in EKMA simulations.

The first series of model simulations performed as part of the present study illustrates the sensitivity of EKMA model predictions to daily loading of isoprene emissions, where daily loading refers to the total amount of isoprene emitted during the simulation. For these tests, the total isoprene loading was varied from 0 to 50 kg/km^2, with the hourly emission rates determined according to the distribution shown in Figure 1. EKMA model predictions have been plotted as a function of the total isoprene loading in Figure 2. The top portion of that figure shows model predictions of peak ozone, whereas the bottom portion shows the model predicted VOC and NO_x control estimates. It is apparent from Figure 2 that the EKMA predicted peak ozone does not increase significantly with increases in isoprene emission loading. Over the entire range considered here, the increase is less than 20%. The bottom graph shows, however, that VOC control estimates increase rapidly with increases in the isoprene emission loading. For an isoprene loading of about 40 kg/km^2 or more, the model predicts that complete elimination of all anthropogenic VOC emissions will not be sufficient to lower the peak ozone concentration to 0.12 ppm. The NO_x control estimates decrease gradually with increased isoprene emission loading, dropping from 55% to 38% over the range considered here. Note that the same degree of VOC and NO_x control is predicted at a total isoprene loading of about 10 kg/km^2.

To illustrate the relative importance of the timing of the post-0800 emissions, a second set of simulations was conducted in which the number of hours during which isoprene is emitted was increased consecutively from zero to eleven. The isoprene emission rate for each hour corresponds to the hourly

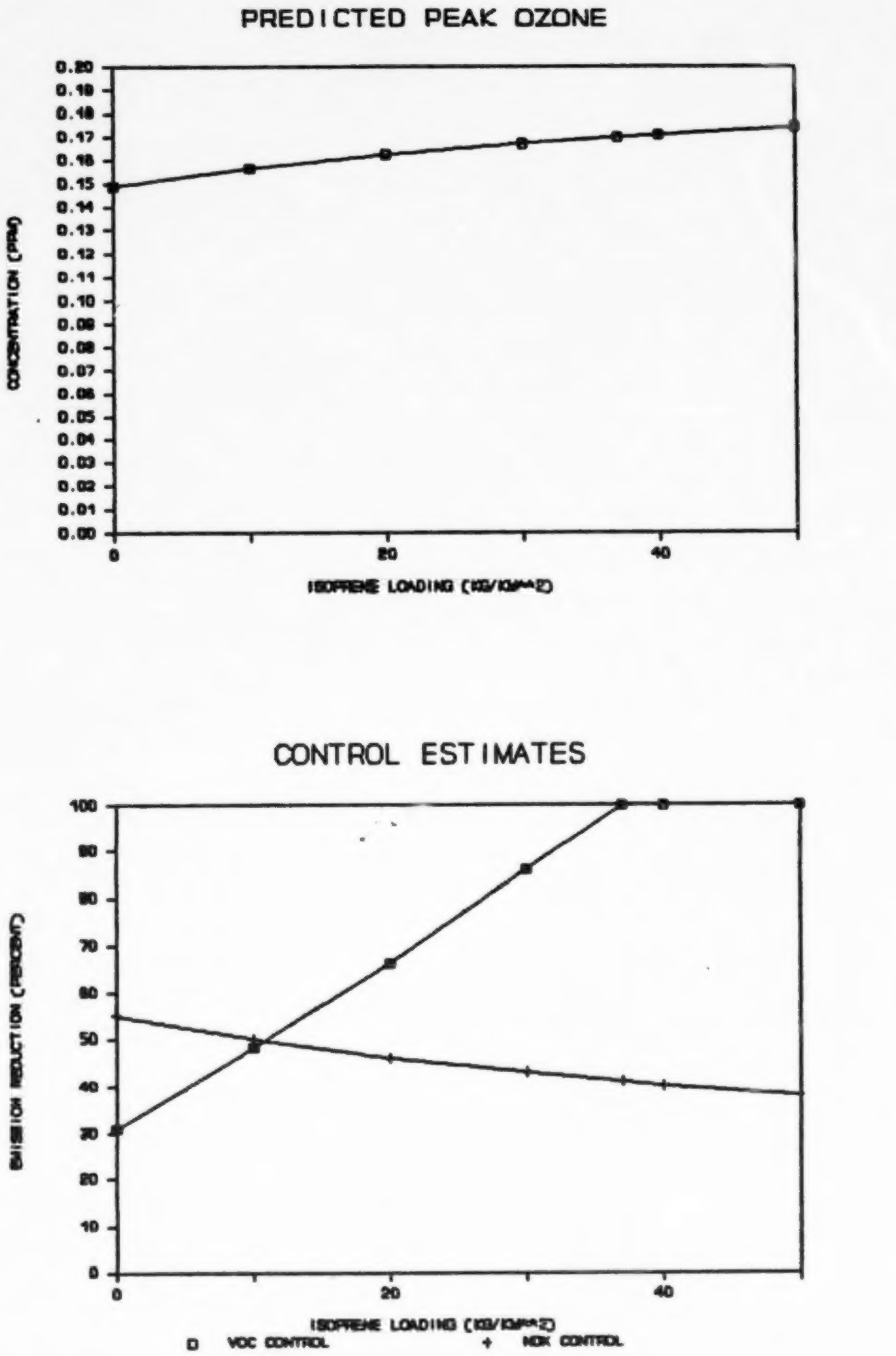
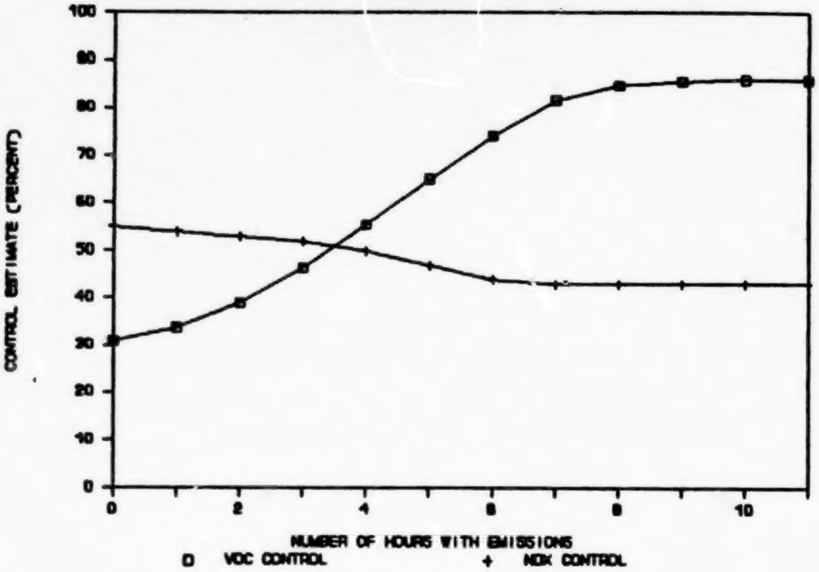


Figure 2. Sensitivity of EKMA model predictions to isoprene loading.

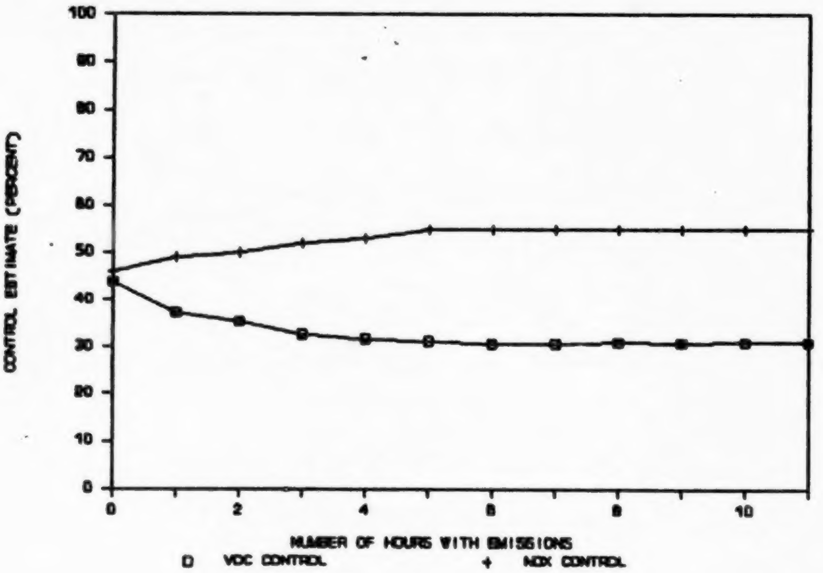
value obtained using the 30 kg/km^2 daily loading and the diurnal distribution shown in Figure 1. The VOC and NO_x control estimates obtained from these simulations are displayed graphically in the top portion of Figure 3 as a function of the number of hours of post-0800 isoprene emissions. For comparison, the bottom portion of Figure 3 shows control estimates obtained without including isoprene emissions plotted as a function of the number of hours of post-0800 anthropogenic emissions. For the simulations with isoprene, emissions occurring up to about the eighth or ninth hour affect control estimates at least to some degree. When only anthropogenic emissions are included in the simulations, however, emissions after about the third or fourth hour have virtually no effect on the control estimates. This is at least to be partially expected since the anthropogenic emissions tend to decrease throughout the simulation, whereas the isoprene emissions are still at their highest levels seven hours into the simulation. Nevertheless, these results indicate that isoprene emitted late in the afternoon may have some effect on control estimates if the emissions rates are near the magnitude assumed here.

OTHER ATLANTA EPISODES

The tests described thus far consisted of simulating a single episode or exceedence of the ozone NAAQS. As part of the SIP for Atlanta, a total of twelve different exceedences of the ozone NAAQS were analyzed. Table 1 lists the date of occurrence, the monitoring site location, and the observed ozone peak for each exceedence (Baugues, 1989). To test the effects of isoprene emissions across a wider range of conditions, the exceedences in Table 1 were



VARIATIONS IN ISOPRENE EMISSIONS



VARIATIONS IN ANTHROPOGENIC EMISSIONS

Figure 3. Sensitivity of EKMA control estimate predictions to the timing of post-0800 emissions.

Table 1

Exceedences Modeled in Atlanta SIP[1]

DATE	Monitoring Site	Measured O_3 Maximum, ppm
7/18/86	Decatur	0.164
7/23/86	Decatur	0.164
6/26/86	Decatur	0.163
6/27/86	Decatur	0.160
7/31/86	Decatur	0.152
4/26/86	Decatur	0.142
6/26/86	Conyers	0.165
7/10/84	Conyers	0.155
6/04/84	Conyers	0.147
8/22/84	Conyers	0.147
6/26/85	Conyers	0.145
7/12/85	Conyers	0.145

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[1] Source: Baugues, 1989

modeled both with and without isoprene emissions as part of this effort. For the simulations with isoprene, the same basic assumptions made by Chameides et al. were used: namely, a total isoprene loading of 30 kg/km_2 is assumed, with the diurnal distribution shown Figure 1. The other EKMA model inputs for these cases were derived from information contained in the Atlanta SIP, and are listed in Appendix D.

Of the twelve exceedences listed in Table 1, EKMA solutions could not be found in five cases (i.e., the given VOC/NO_x ratio line did not intersect the isopleth corresponding to the observed ozone peak). No attempt was made to resolve the problem, and these cases were eliminated from further consideration. The modeling results for the remaining exceedences (except the June 4, 1984 exceedence at Conyers discussed above) are presented in Figure 4 as a series of clustered bar graphs showing VOC and NO_x control estimates both with and without isoprene emissions included. In these graphs, several VOC control estimates are shown as 100%. In actuality, the model simulations for these cases indicated that the elimination of all anthropogenic VOC emissions is insufficient to reduce peak ozone to 0.12 ppm.

The results for these additional analyses are similar to those found for the June 4, 1984 exceedence discussed previously. When isoprene emissions are added to the simulations, VOC control estimates increase drastically, whereas NO_x control estimates tend to decrease somewhat. In all cases but one, the VOC control estimate is lower than the NO_x control estimate when isoprene emissions are omitted from the simulations. But when isoprene emissions are included, the NO_x control estimate is substantially lower than the

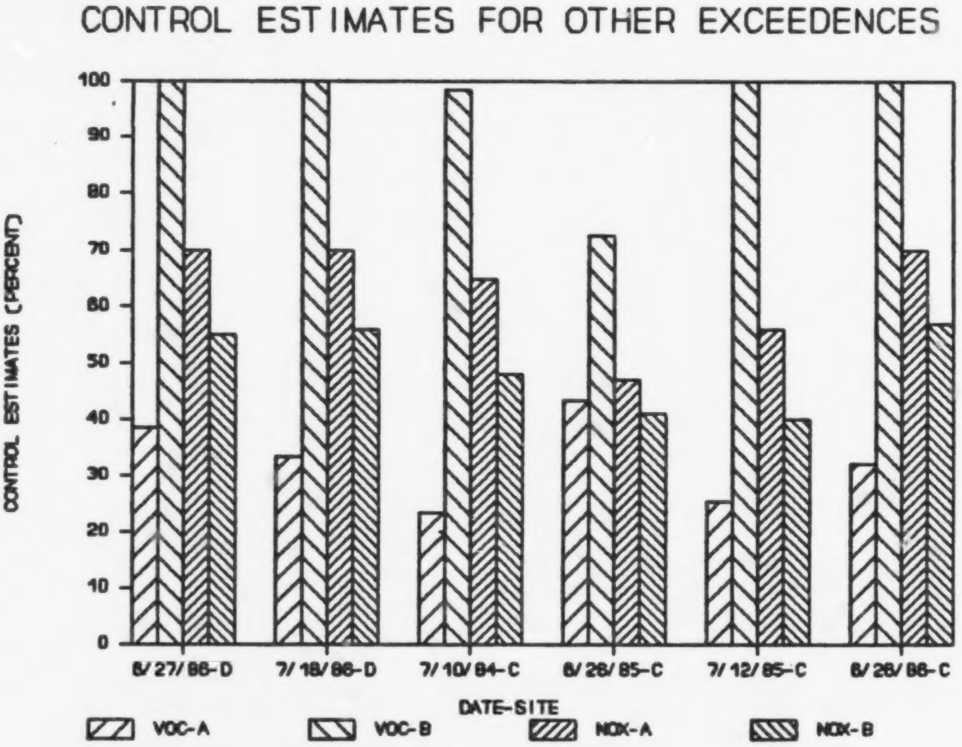

Figure 4. EKMA predictions of VOC and NOX control estimates for other Atlanta exceedences. (A-anthropogenic emissions only, B-isoprene emissions included, C-Conyers monitoring site, D-Decatur monitoring site)

corresponding VOC control estimate. The latter finding is consistent with that obtained by Chameides et al. in their analysis of the June 4, 1984 exceedence.

MISCELLANEOUS TESTS

As described above, a number of different exceedences were modeled to asses the effect of isoprene emissions over a wider range of conditions than the single June 4, 1984 exceedence. Although some of the EKMA model inputs do vary from case to case, other model inputs varied very little or not at all. For example, the VOC/NO_x ratio is the same for all cases, the same reactivity for anthropogenic emissions was used in all cases, and in only one case did the mixing heights vary significantly. This subsection describes the results of sensitivity tests that were conducted by systematically varying selected EKMA model inputs to assess the impact of biogenic emissions under a broader range of conditions. It should be emphasized that some of the variations in model inputs considered here may not necessarily be representative of conditions in Atlanta, but may be appropriate for some other areas of the country. Further, the results obtained using these inputs may provide additional information on key variables that could affect the impact of biogenic emissions.

All of the simulations discussed below were performed using the revised model inputs for the June 4, 1984 exceedence that was discussed above. Since the biogenic emissions have the greatest effect on VOC control estimates, only they are considered here. As was done in previous tests, all simulations that include biogenic emissions have been made using a total daily loading of 30 kg/km^2/day of isoprene and distributed hourly according to Figure 1. The other EKMA inputs were varied one at a time, so compound effects are not considered here.

The results of the sensitivity tests are shown in Table 2, grouped according to the model input variable that was varied. Explanations on the derivations of some of the model inputs are included as footnotes in the table. For reference, the first entry in each group corresponds to the results obtained using the revised model inputs that are listed in Appendix C and were discussed earlier (i.e., the basic inputs for Atlanta). Consider first the results obtained when biogenic emissions are omitted. Only two of the inputs considered here significantly affect the VOC control estimates - the VOC/NO_x ratio and the variation of the post-0800 emissions. Although the variations considered here resulted in increases in the VOC control estimates, they are still significantly lower than the corresponding estimates obtained with isoprene emissions included. For the cases in which isoprene emissions are included, the only variable of those considered here that significantly affects the VOC control estimates is the maximum afternoon mixing height. As might be expected, the impact of isoprene emissions is lessened as the mixing height is increased. Nevertheless, even at the highest mixing height considered here (2500 meters), the impact of isoprene emitted at the assumed rate of 30 kg/km^2/day is substantial.

Table 2

Sensitivity of Biogenic Impacts to Variations in Selected EKMA Inputs

Description	VOC Control Estimates (%) W/O Isoprene	 W/ Isoprene
I. VOC/NOx Ratio		
VOC/NOx = 7	31	86
VOC/NOx = 10	48	88
VOC/NOx = 15	61	90
II. Dilution		
Maximum afternoon mixing height = 1500m	31	86
Maximum afternoon mixing height = 2000m	30	71
Maximum afternoon mixing height = 2500m	30	62
III. Reactivity[1]		
Default	31	86
1984 ambient measurements	34	86
1986 ambient measurements	33	86
IV. Post-0800 Emissions[2]		
Revised inputs based on SIP	31	86
Anthropogenic VOC emissions doubled	42	88
V. Temperature[3]		
Default	31	86
Observed profile	32	87

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[1] Reactivity of anthropogenic VOC derived from ambient measurements of VOC species taken in Atlanta in 1984 and 1986 (Jeffries et al., 1987)

[2] Included to simulate the effects of a potential underestimation of VOC emissions from anthropogenic sources.

[3] Temperature profile derived from Atlanta Local Climatological Data (LCD) report for June 4, 1984.

SECTION 3

USE OF A DETAILED BIOGENIC EMISSION INVENTORY

The sensitivity tests described in the preceding section were performed using biogenic VOC emission rates based on the regional, average estimates of Chameides et al., with all the biogenic VOC emissions represented as isoprene. This section describes a series of sensitivity tests conducted for the Atlanta region that make use of biogenic emission estimates from an inventory that is more highly resolved spatially and temporally than the one used previously. In addition, biogenic emissions of species other than isoprene are also considered. Thus, the tests that are described here are made using different assumptions on the magnitude and diurnal variation in biogenic VOC emissions, as well as on the chemical composition of the biogenic organics. As before, the major focus of these tests is on quantifying the impact of including biogenic VOC emissions on both VOC and NO_x control estimates.

As part of EPA's ongoing effort to develop and apply the Regional Oxidant Model (ROM), a gridded, hourly biogenic VOC emission inventory has been developed (Novak and Reagan, 1986). One portion of that inventory encompasses the Atlanta metropolitan region, and it has been used to develop biogenic emission inputs for the EKMA applications described below. Each of the ROM inventory grid cells is 1/4 degree longitude by 1/6 degree latitude, which for the Atlanta region represents a grid cell that is about 23 km wide by 18.5 km high. For the ROM inventory, biogenic emissions have been compiled for individual species or groups of species, and then apportioned to the CB-4 functional groups ISOP, PAR, and OLE according to chemical composition. Empirical relationships have been used to adjust emission rates of individual species to account for variations in temperature and light intensity, two factors which affect biogenic emission rates. A complete description of the specific procedures used to develop the inventory is contained in the paper by Novak and Reagan.

Figure 5 has been prepared to illustrate the spatial distribution of biogenic emissions in the vicinity of the Atlanta metropolitan area using information that is available in the ROM emissions inventory. In this figure, each square represents a ROM grid cell, with the Atlanta urban core located in the center grid. The total land area encompassed by all 25 grid cells is approximately 11,000 km^2. The entries in each square show daily loadings (i.e., the sum of emissions from 0800-1900 LDT as used in this report) of both isoprene and total biogenic VOC emissions within the cell for a single day (July 10,1980). Biogenic VOC emissions for this particular day should be relatively high since the maximum afternoon temperature recorded at the Atlanta airport was 99 degrees F and clear sky conditions existed for most of the day. For ease of comparison with the assumptions made by Chameides et al., the emissions in the ROM inventory have been converted to mass emission densities (i.e., kg/km^2) in Figure 5. Recall from previous discussions that the region-wide estimates of Chameides et al. corresponding to this time period are 50 kg/km^2 for total biogenic VOC and 30 kg/km^2 for isoprene. To illustrate the temporal distribution of the biogenic emissions, Figure 6 is a plot showing the fraction of the total daily loadings of isoprene and non-

16 ---- 39	11 ---- 64	20 ---- 54	21 ---- 56	24 ---- 54
21 ---- 57	9 ---- 49	7 ---- 26	13 ---- 45	16 ---- 37
21 ---- 57	22 ---- 60	3 -X- 8	8 ---- 41	15 ---- 34
21 ---- 58	13 ---- 52	10 ---- 47	14 ----C 53	17 ---- 39
22 ---- 58	13 ---- 53	20 ---- 52	20 ---- 53	25 ---- 59

X = Atlanta center-city   C = Conyers monitor

Figure 5. Schematic representation of ROM emission inventory grid network in the vicinity of Atlanta. [The top entry in each cell is the total daily loading of isoprene emissions, and the bottom entry the loading of total biogenic VOC (kg/km^2) for July 10,1980.]

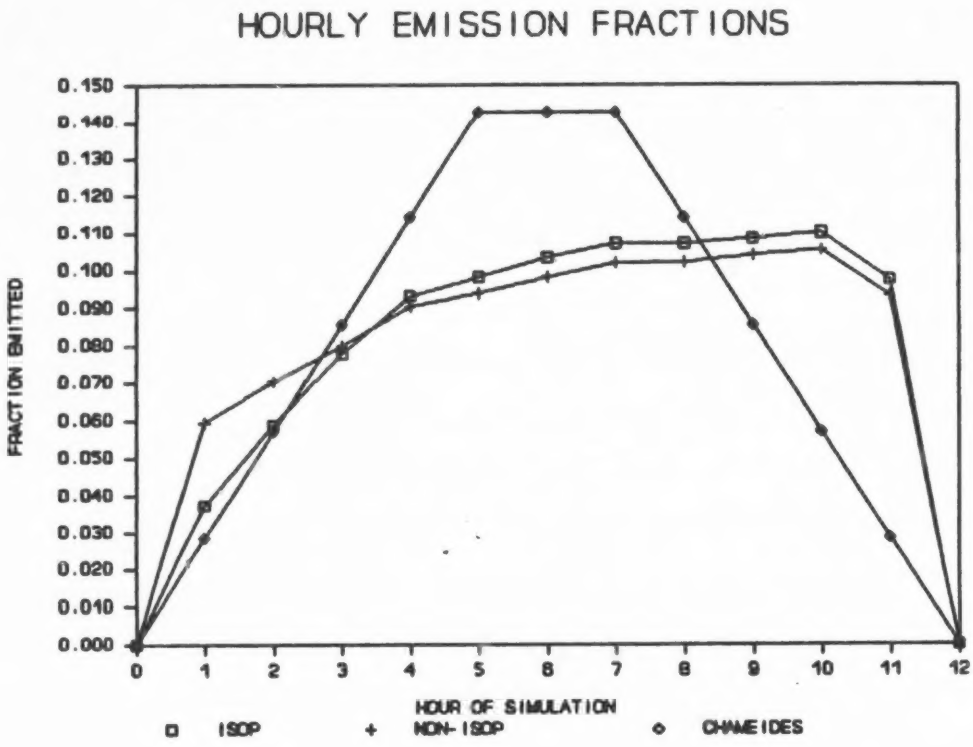

Figure 6. Example diurnal distribution of isoprene and non-isoprene emissions from ROM inventory compared to the assumption of Chameides et al.

isoprene VOC emitted each hour for the cell containing the Conyers monitor, along with the diurnal distribution assumed by Chameides et al.

As noted above, the biogenic compounds in the ROM inventory are represented in the CB-4 mechanism as ISOP, PAR, and OLE. From Figure 5, it is apparent that the portion of the total biogenic VOC that is isoprene varies from cell to cell, ranging from a low of 20% to a high of 45% on a mass basis. The non-isoprene portion of the biogenic VOC represents emissions of monoterpenes and other unidentified compounds, which are represented in the CB-4 by the PAR and OLE functional groups. On a mass basis, approximately 20% of these emissions are represented by the OLE functional group. In the simulations that are described below, therefore, the biogenic VOC emissions are modeled using three different CB-4 functional groups to represent emissions of isoprene, monoterpenes, and other unidentified compounds.

In the simulations that are discussed below, two different approaches are employed to use the information in the ROM biogenic emission inventory for the EKMA modeling applications. In the first, spatially averaged emission estimates of biogenic VOC are used as before, but variations in the extent of the area of coverage are considered. In the second approach, a trajectory analysis concept is used that incorporates both spatial and temporal variations in biogenic emissions. As before, the June 4, 1984 exceedence is modeled using the revised inputs included in Appendix C. Since biogenic emissions from the ROM inventory are not available for this particular day, and since biogenic emissions can be relatively sensitive to temperature variations, emissions from two different days are included in the analyses described below. The day with the higher emissions (July 10, 1980) had a maximum temperature of 99 degrees F as compared to 90 degrees F for the other day (August 26, 1980). It should be noted that the maximum temperature for the June 4, 1984 exceedence was only 89 degrees F, so emissions for the day with the lower temperature may be more appropriate for modeling this particular exceedence. Nevertheless, maximum temperatures on days of other exceedences in Atlanta approached 100 degrees F, so it is conceivable that the higher emissions corresponding to a warmer day may be more appropriate in some instances. In the discussions that follow, the biogenic emissions for the day with the higher temperature will be referred to as the high emission case, whereas those for the other day will be referred to as the moderate emission case.

SPATIAL AVERAGING APPROACH

Three levels of geographic coverage are considered in developing the spatially averaged estimates of biogenic VOC emissions from the ROM inventory for use in the EKMA simulations that are described here. In the first level, only emissions from the cell including the urban core are used (i.e., the center cell in Figure 5). Biogenic emissions are lowest in this cell and are presumably most representative of emissions in an urban area. The use of these emission estimates may be most appropriate for modeling exceedences that are detected at monitors located relatively close to the urban core. (Note that in the Atlanta region, the Decatur monitoring site is located in the same ROM grid cell as the urban core, and exceedences of the NAAQS were detected at this site as well as the Conyers site currently being considered.) Further, model predictions obtained with these emissions may provide some indication of the lower bound of the potential effects of including biogenic emissions in EKMA simulations since they are lowest in this cell. The other two levels of spatial averaging are relatively arbitrary symmetrical expansions about the center grid containing the Atlanta urban core. Biogenic emissions have been averaged across the nine cells immediately surrounding and including the urban core, as well as all of the 25 cells shown in Figure 5. Table 3 lists the total daily loadings of the biogenic VOC for the two emission days and the three levels of spatial averaging considered here.

The EKMA modeling results obtained using the three different spatially averaged emission estimates are depicted graphically in the clustered bar graphs shown in Figure 7. For reference, the first bar in each cluster shows the control estimate obtained for the case in which biogenic VOC emissions are not included in the simulation. The control estimates for the next three bars are the results obtained using the single-cell, 9-cell, and 25-cell average biogenic emission estimates, in that order. Since the biogenic emissions increase with the area of coverage, the progression from left to right in these graphs reflects increases in biogenic emissions, although the incremental increases are not uniform.

The pattern of results obtained here parallels that found in the preceding section, though the impacts themselves are somewhat less in most cases. The NO_x control estimates tend to decrease with increases in the biogenic emissions, but those decreases are relatively small. VOC control estimates again increase appreciably with biogenic emissions, although for

Table 3

Biogenic Emission Estimates Using the Spatial Averaging Approach[1] (kg/km^2)

I. High Emission Case (July 10,1980)

	1-Cell	9-Cell Average	25-Cell Average
ISOP	3.3	11.0	16.1
PAR	3.9	25.0	25.7
OLE	1.0	6.3	6.4
TOTAL	8.2	42.3	48.2

II. Moderate Emission Case (August 26, 1980)

	1-Cell	9-Cell Average	25-Cell Average
ISOP	1.9	6.2	9.0
PAR	2.8	17.8	18.3
OLE	0.7	4.4	4.6
TOTAL	5.4	28.4	31.9

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[1] All estimates were derived from the ROM biogenic emission inventory.

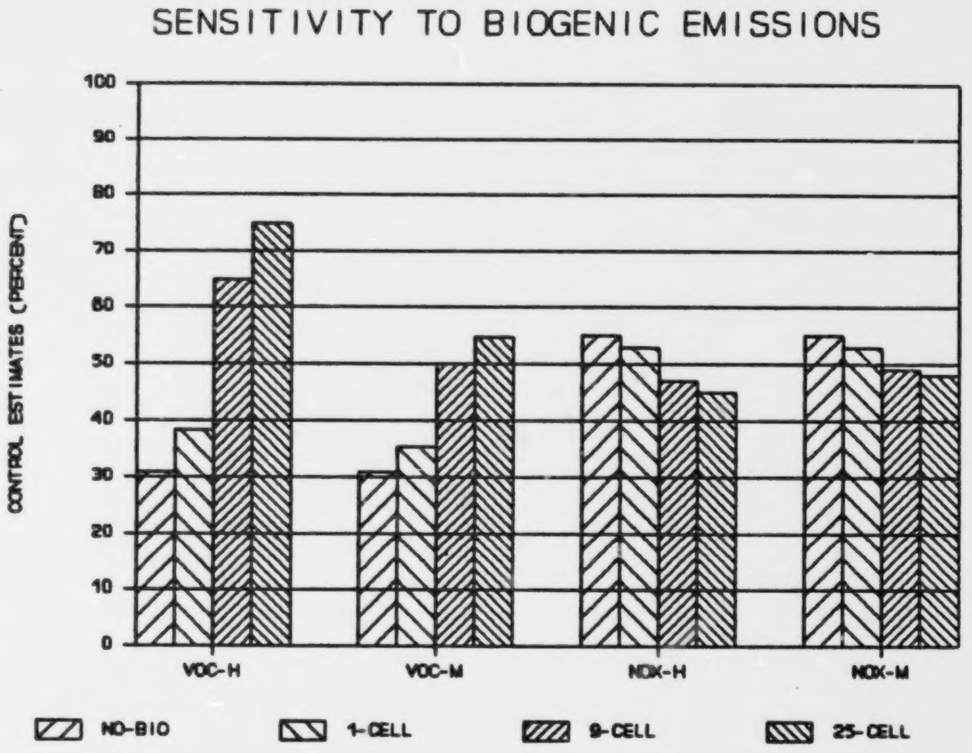


Figure 7. Control estimates obtained using spatially averaged, biogenic emission estimates. (H-High biogenic emissions case, M-Moderate biogenic emissions case)

most cases the increases are more moderate than found using the Chameides et al. assumptions regarding isoprene emissions. Nevertheless, the increases found with the 9-cell and 25-cell average emissions for the high emissions case are close to the 70% control estimate reported by Chameides et al. Also, the NO_x control estimates found with the 9-cell and 25-cell averages are lower than their corresponding VOC control estimates for both the high and moderate emission cases. Finally, as noted above, use of the single-cell average may provide at least some indication of the minimal impact of including biogenic VOC emissions in EKMA simulations for Atlanta. For the high emissions case, the VOC control estimate is 7% higher than the one for the case in which biogenic emissions are ignored (i.e., 38% versus 31%). For the moderate biogenic emission case, the increase is only 4% (i.e., 35% versus 31%).

TRAJECTORY ANALYSIS APPROACH

The current EPA guidelines for applying EKMA recommend that it be applied using a simplified, straightline trajectory in which ozone formation is simulated in a column of air travelling at uniform speed from the center city to the site of the observed ozone maximum (EPA, 1987). Post-0800 emissions from anthropogenic sources are estimated at each hour by the location of the column and the available spatial and temporal resolution of the emission inventory. Typically, emission inventories are resolved only to the county level, but a finer, gridded inventory may be used when available. In this section, the trajectory approach is used to define the post-0800 VOC emissions from anthropogenic and biogenic sources using the ROM emission inventory.

With the ROM grid network, the straightline EKMA trajectory from the urban center to the Conyers monitoring site would originate in the center cell in Figure 5, pass through the cell to the immediate right of the center cell for a brief period, and then enter the cell below. Rather than focus on a single trajectory in this analysis, however, the approach taken is to evaluate the sensitivity of the model predictions to the number of hours the air column is assumed to be in the grid cell containing the center-city. The post-0800 biogenic emissions are derived by using emissions for the center grid cell for a chosen number of hours, using the emissions for the grid to the immediate right for the next hour, and then finally using emissions for the grid that contains the Conyers site for the remaining hours of the simulation. Residence time in the grid cell containing the center-city is varied from three to six hours. The other EKMA model inputs correspond to the revised EKMA inputs in Appendix C (i.e., the June 4, 1984 exceedence). Not only does this type of analysis provide information on the sensitivity of the results to the specific trajectory assumed here, but it also may provide some indication of the effect that variations in wind speeds and city size may have on the impact of biogenic emissions as well. For the latter case, the longer residence times in the center city grid would correspond to lower wind speeds and larger urban areas.

Figures 8 and 9 show the total daily loadings of isoprene and total biogenic VOC emissions and the model predictions of VOC and NO_x control estimates found using each of the assumed trajectories described above. Both the biogenic emissions and the control estimates have been plotted as a function of the number of hours the air column is assumed to remain in the

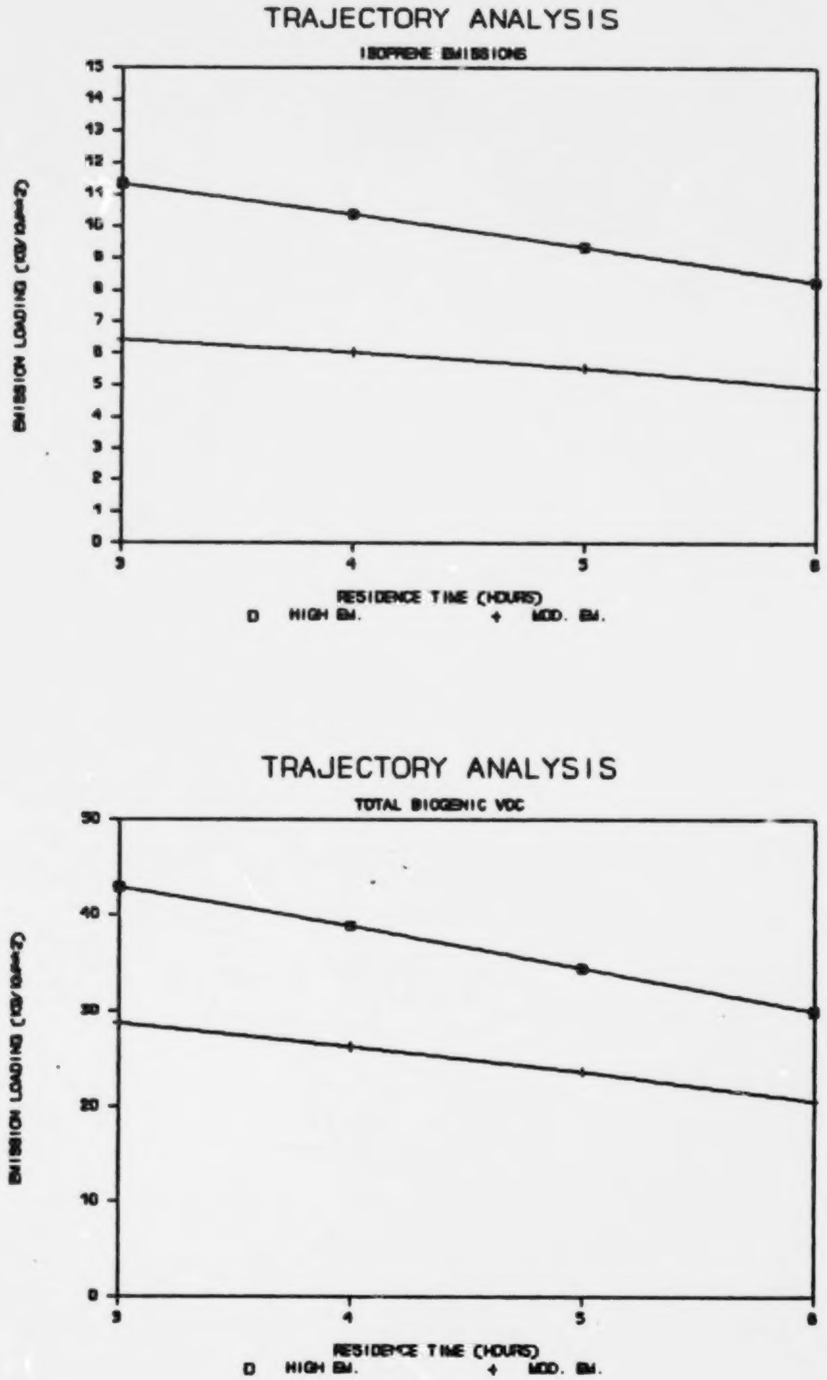
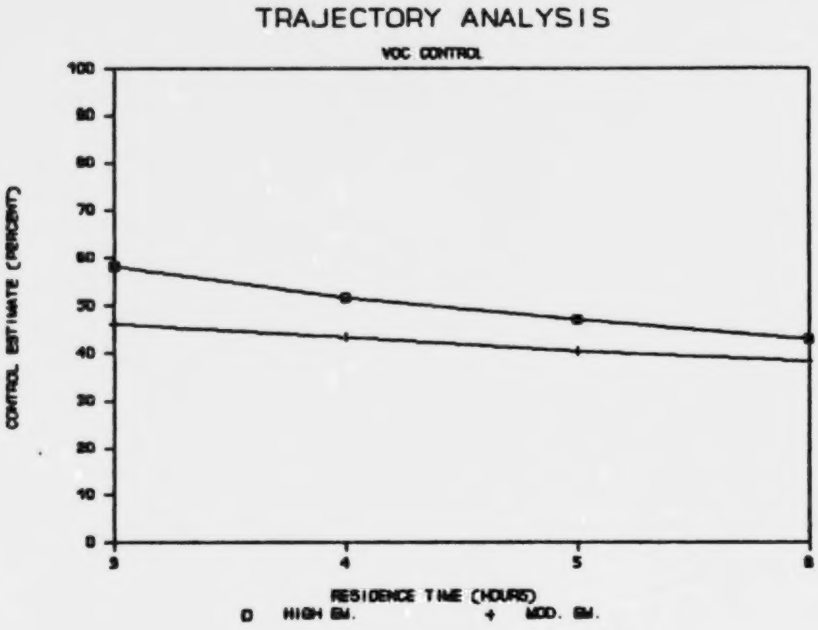


Figure 8. Post-0800 biogenic emissions as a function of center-city grid cell residence time.



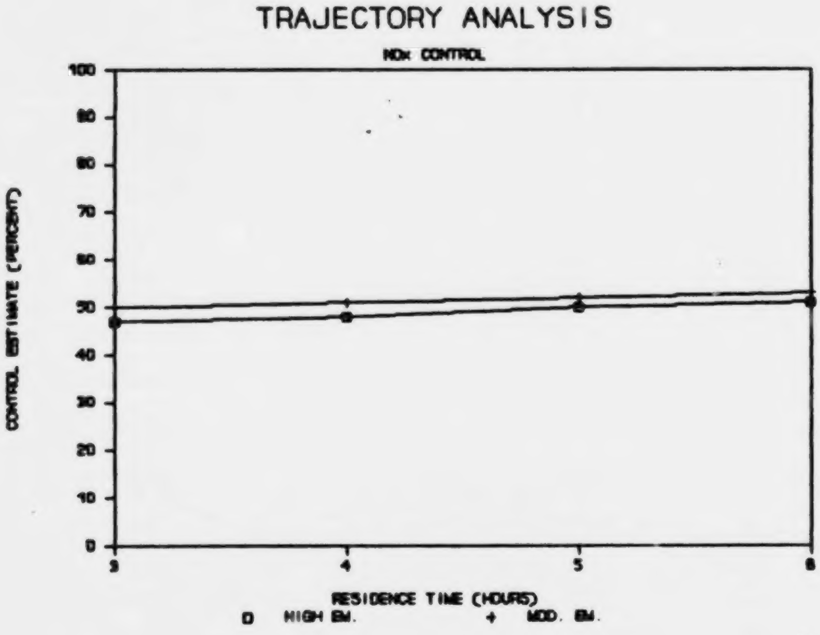


Figure 9. VOC and NOx control estimates calculated for the trajectory analysis as a function of center city grid cell residence time.

center grid. As shown in Figure 9, both the isoprene and total biogenic VOC loadings decrease with increasing residence time. It should be noted that the biogenic emission rates in the morning hours and early afternoon hours are also being changed significantly. Thus, the control estimates shown in Figure 10 are due not only to changes in total daily loading but also to changes in the timing of the biogenic emissions. As shown was shown in Figure 3, the emissions for the first 6 to 7 hours are most likely to have the greatest impact on control estimates.

As seen in Figure 10, the VOC control estimates decrease with increasing residence time within the grid cell containing the center city. The range in VOC control estimates is 43% to 58% for the high biogenic emission case, and 38% to 46% for the moderate biogenic emission estimates. These impacts are lower than those found by Chameides et al., but still appreciably higher than the 31% VOC control estimate obtained without including biogenic emissions. Finally, the NO_x control estimates decrease very little with increases in residence time, and exceed the corresponding VOC estimates for all but the high biogenic emissions case with the two shortest residence times (i.e., 3 and 4 hours).

In the tests described above, the post-0800 anthropogenic emissions were held constant while the biogenic emissions were varied. To evaluate the effect of varying both biogenic and anthropogenic emissions in the trajectory analysis approach, the sensitivity tests described above were repeated using the anthropogenic emission estimates from the ROM emission inventory. (Insufficient information was available from the SIP to derive the anthropogenic emission data necessary for this type of analysis). The ROM anthropogenic emissions are for the year 1980, and are considerably higher than those used in the SIP. The total daily loadings of the post-0800 anthropogenic emissions for all trajectories considered here are shown in Table 4. The VOC and NO_x control estimates obtained for these trajectories are plotted as a function of residence time in Figure 10. One curve is included for the case in which biogenics are ignored, and one each for the two biogenic emission cases. With these simulations, VOC estimates decrease with increasing residence time for the case in which biogenics are omitted, as well as for the other two cases. The VOC control estimates for the high biogenic emission case average about 25% higher than the estimates with no biogenics (e.g., 45% versus 20%). The average differential for the low emission case is about 15%. Again, these impacts are somewhat lower than those estimated by Chameides et al. It is also interesting to note that in these simulations, the NO_x control estimates increase more significantly with increasing residence time than in the previous trajectory simulations. This is most likely due to the significant increase in anthropogenic NO_x emissions at the relatively low VOC/NO_x ratio of about 4:1 (see Table 4).

Table 4

Anthropogenic Emission Loadings Used in the Trajectory Analysis Approach[1] (kg/km^2)

Description	VOC	NO_x	VOC/NOX[2]
June 4, 1984 SIP	41.3	36.2	3.6
ROM inventory, 3-hour residence time in center city grid	68.5	53.3	4.1
ROM inventory, 4-hour residence time in center city grid	88.5	68.7	4.1
ROM inventory, 5-hour residence time in center city grid	108.8	85.1	4.1
ROM inventory, 6-hour residence time in center city grid	129.5	101.5	4.1

---

[1] Total anthropogenic emissions for the 11-hour simulation

[2] Molar Basis

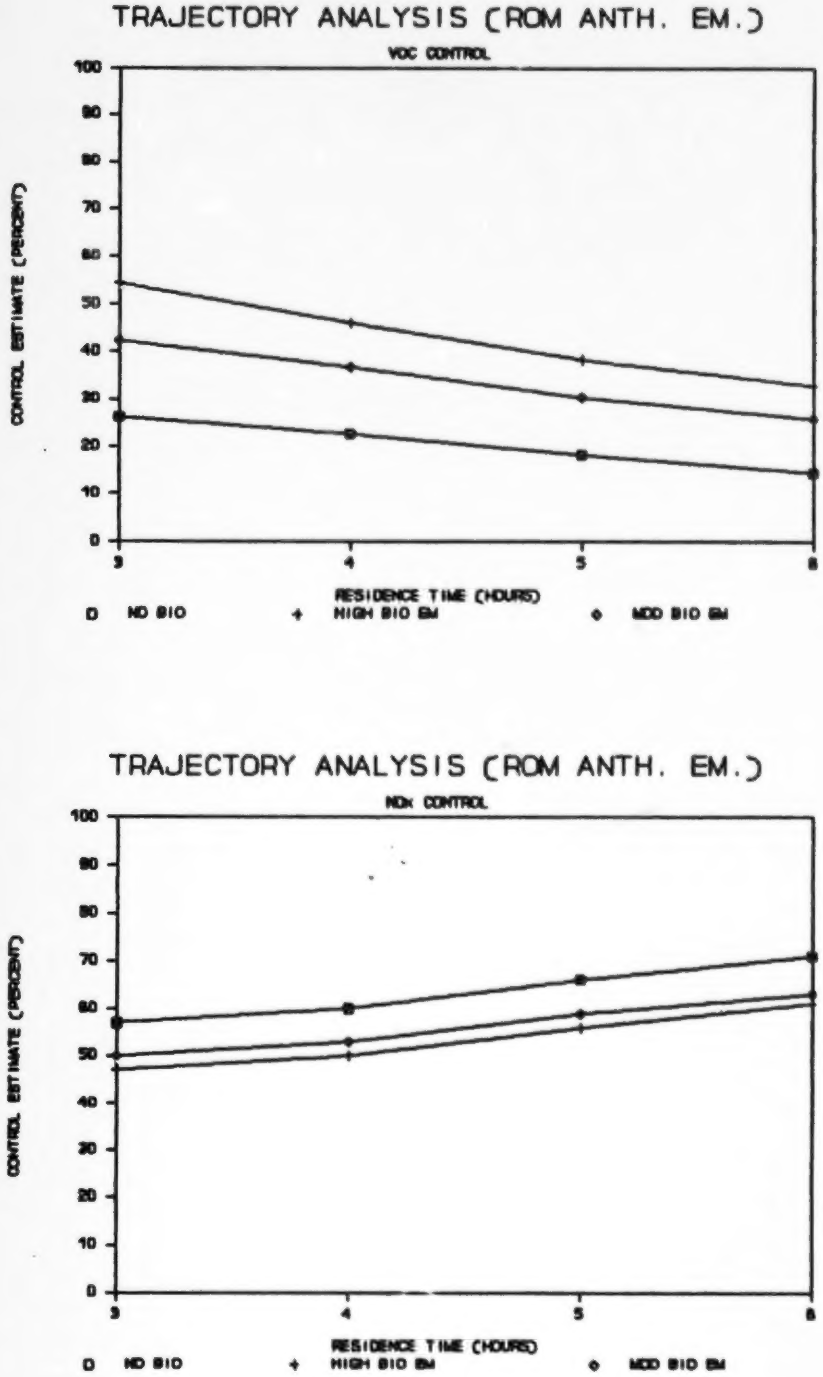


Figure 10. VOC and NO_x control estimates calculated for the trajectory analysis as a function of center city grid cell residence time. (Anthropogenic post-0800 emissions from ROM inventory.)

SECTION 4

POTENTIAL IMPACT OF BIOGENIC EMISSIONS IN OTHER CITIES

The sensitivity of the EKMA model predictions to biogenic emissions has been demonstrated in the previous two sections. It is apparent from these results that VOC control estimates are very sensitive to isoprene emissions, but somewhat less sensitive to emissions of the other biogenics as represented in the CB-4 mechanism in this study. For example, using the 30 kg/km^2 isoprene emission loading estimated by Chameides et al., the VOC control estimate found with the revised EKMA inputs, as described in Section 2, is 86%. In Section 3, the 30 kg/km^2 isoprene loading was replaced with a total biogenic loading of 48 kg/km^2, of which only 16 kg/km^2 is isoprene, and the VOC control estimate dropped to 74%. Thus, even though more biogenic emissions were included in the simulation, the reactivity associated with those emissions was less than that found with the emissions of isoprene alone. As a consequence, a preliminary assessment of the impact of biogenic emissions in other areas can be gained by comparing the isoprene emissions in those areas with the emissions in Atlanta.

Biogenic emission estimates have been compiled from the ROM emission inventory for the following six cities: Houston, Baton Rouge, New York City, Philadelphia, Baltimore, and Pittsburgh. The spatial averaging approach has been used to obtain estimates of the emissions in the urban area, as well as the surrounding region (using the 9- and 25-cell averages as described in the preceding section). Some caution should be used in interpreting these emission estimates, however, since for some cities the center city may not be centrally located in a ROM grid cell, and some of the surrounding grids may include large areas with virtually no biogenic emissions (e.g., large bodies of water). Nevertheless, the emission estimates presented in this manner should provide at least some indication of the relative magnitude of biogenic emissions in the vicinity of these cities as compared to Atlanta.

Figure 11 shows both isoprene and total biogenic VOC emissions for the period 0800-1900 LDT for the six cities and Atlanta for the day with relatively moderate temperatures. For the two southern cities, the emissions are for the moderate emission day used previously for Atlanta. The maximum afternoon temperature of 92 degrees F in Baton Rouge for that day was comparable to that in Atlanta, but it was significantly higher in Houston (98 degrees F). For the northeastern cities, the biogenic emission estimates are for July 14, 1980, for which the maximum temperatures in these cities were in the upper eighties, again comparable to the Atlanta emission case. As shown in Figure 11, both isoprene and total biogenic VOC emissions in the vicinity of Baton Rouge are higher than the emissions in Atlanta for this particular case. Emissions for all of the other cities are lower than those for Atlanta. As a result, it is likely that including biogenic emissions in EKMA applications for the cities other than Baton Rouge is likely to have less of an impact than for Atlanta applications. Impacts in Baton Rouge may be comparable to those in Atlanta, depending on other factors such as the VOC/NO_x ratio, mixing heights etc.

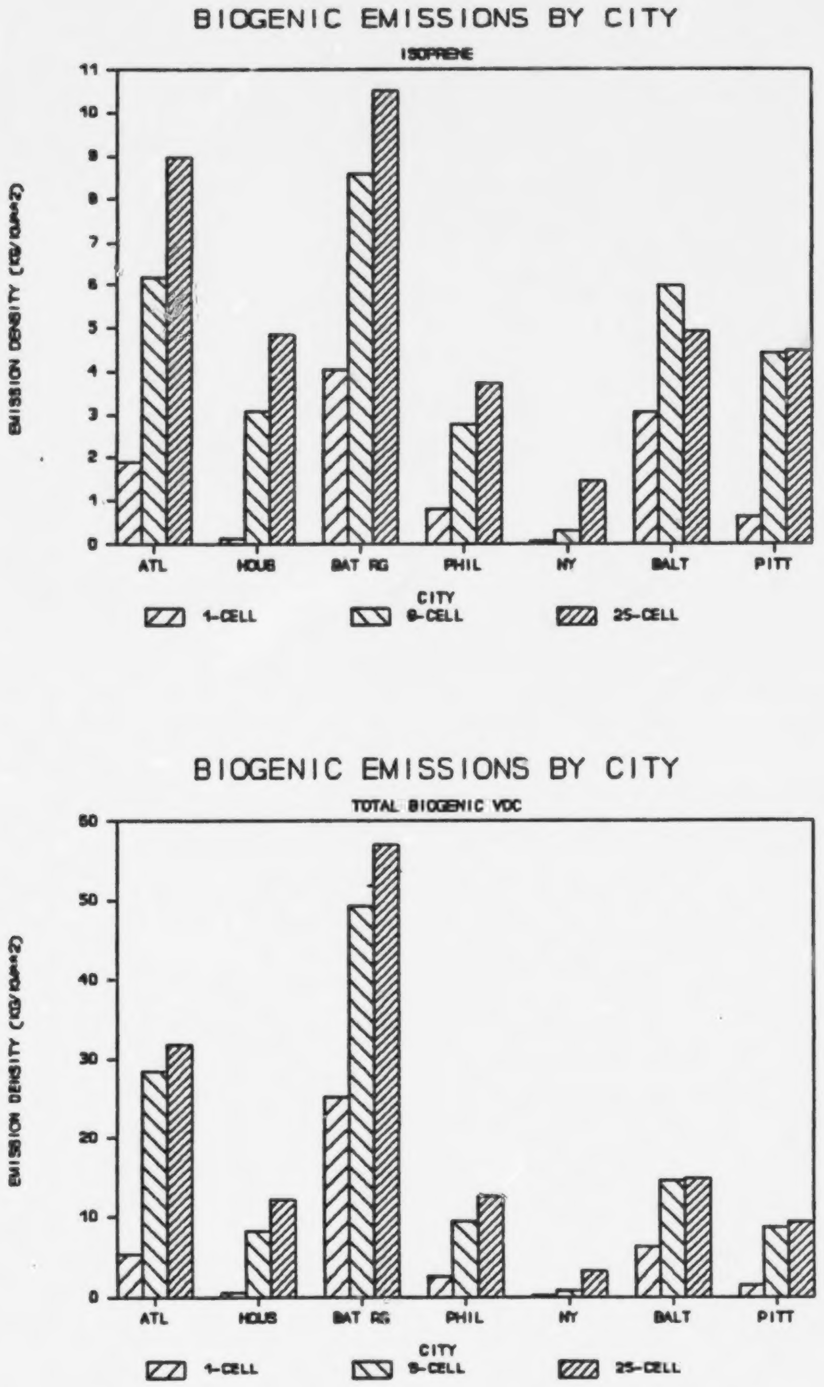


Figure 11. Estimates of biogenic emissions in other cities.

SECTION 5

SUMMARY OF RESULTS

In the analysis performed by Chameides et al., the inclusion of biogenic emissions was found to have a substantial impact on the estimated reductions in VOC emissions from anthropogenic emissions that would be required to attain the ozone NAAQS. For the particular application they considered, the VOC control estimate increased from 30 to 70 percent when biogenic emissions were included in the EKMA simulations. As noted in their article, the VOC control estimate was found to be greater than the NO_x control estimate whenever isoprene emissions are greater than about 30 kg/km^2. As a consequence, they conclude that it is essential to include the effects of biogenic emissions in developing control strategies for reducing ambient ozone concentrations.

The sensitivity tests described in Section 2 of this report essentially lead to the same findings as those of Chameides et al. Using the same basic assumptions, with some minor adjustments to the EKMA model inputs, the VOC control estimate was found to increase from 31% to 86% when biogenic emissions are added. The NO_x control estimate for the case with biogenics was found to be 43%, substantially lower than the corresponding VOC control estimate of 86%. Additional tests described in that section demonstrated that the VOC control estimates are critically sensitive to the total isoprene loading, that emissions of isoprene throughout most of the simulation period affect VOC control estimates, and that similar results are found for other Atlanta exceedences. Besides total daily loading of isoprene emissions, the only other EKMA model input that significantly affects the impact of the isoprene emissions is the maximum afternoon mixing height.

In Section 3, the effect of using a more refined spatially and temporally resolved emission inventory for biogenic emissions in EKMA applications was examined. Although regional average estimates of total biogenic VOC in this inventory agree reasonably well with those of Chameides et al., the isoprene emission estimates are somewhat lower. Two approaches were examined for using the greater detailed inventory in EKMA modeling applications, and the manner in which each approach is applied was found to have a significant impact on the EKMA control estimate predictions. For example, if biogenic emissions for the urban area (as represented by the grid cell encompassing the center city) are used solely in the EKMA modeling applications, VOC control estimates are found to increase by less than 10 percent (e.g., 40% versus 30%). If biogenic emissions are averaged across a much broader area, however, the impacts approach those reported by Chameides et al. If a trajectory analysis approach is used, the impacts are somewhere in between, increasing VOC control estimates anywhere from 10 to 30 percent depending on the assumptions made with regard to the trajectory. Finally, the emission estimates in the ROM biogenic emission inventory are quite sensitive to temperature, with emissions on a day with a maximum temperature of about 100 degree F being about twice those on a day with a maximum temperature of only 90 degrees F.

As noted in Section 4, the EKMA model predictions are more sensitive to isoprene emission estimates than the other biogenic compounds as modeled in the CB-4 mechanism. As a result, a comparison of isoprene emissions in other cities with those in Atlanta should provide some indication of how important biogenic emissions may be in those cities. The ROM emission inventory was used to compile daily isoprene emissions in six cities. Of these six, only Baton Rouge was found to have isoprene emissions greater than those for Atlanta. The northeastern cities that were considered appear to have somewhat lower isoprene emissions than Atlanta, and thus the impacts of biogenic emissions would be expected to be somewhat less than in Atlanta.

The results of the sensitivity tests described above suggest that the role of biogenic emissions should be included in EKMA applications for control strategy development. Although uncertainties exist in making estimates of biogenic emissions, they nevertheless may have a significant affect on modeling applications designed to evaluate control strategy effectiveness. The results also suggest that the EKMA modeling results may be critically affected by the spatial and temporal resolution of the biogenic emissions data used in the modeling applications. If a trajectory approach is used, the possibility exists that significant differences could be found in control estimates by modifying the trajectory only slightly. This problem may be mitigated to some degree if biogenic emissions are compiled with a finer spatial resolution than was considered in this study however. (In the ROM inventory, there are substantial gradients in biogenic emissions between the grid containing the urban area and those surrounding it, leading to large changes emissions as the trajectory passes from the urban grid. These gradients may be lessened if greater spatial resolution is used in the inventory compilation.) Finally, biogenic emissions in the ROM inventory show a strong dependence on ambient temperature. It may thus be necessary to develop methods for accounting for this temperature dependence in EKMA applications in situations where detailed biogenic emission inventories such as the ROM inventory are not available.

SECTION 6

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APPENDIX A

Description of EKMA Procedures Used to Evaluate the Effects of Biogenics

Most of the EKMA model simulations performed as part of this study were made with a special PC version of the OZIPM4 computer program. VOC control estimates were calculated using the EKMA option, for which the VOC/NOX ratio and ozone design values are input and the program computes required VOC reductions. The NOx control estimates were calculated by repeated simulations using the CALC option with NOx levels varied and VOC levels held constant. All other EKMA input variables were held constant in the control calculations.

The nonbiogenic EKMA inputs were used in the standard manner. For the biogenic inputs, the MOLE option was used. With this option, all post-0800 emissions are input in mole units, but only the post-0800 VOC and NOx emissions are varied in the control strategy calculations. Thus, individual species such as ISOP, PAR, and OLE can be input with this option and held constant in the EKMA control calculations. To use this option, it is necessary to specify an initial concentration that is added at the beginning of the simulation. For all biogenic emissions, this concentration was set to a very small number (e.g. 0.00001 ppm) to effectively yield an initial concentration of zero. (An example set of inputs for isoprene emissions is included in Appendix C.) Finally, all conversions between mass and moles have been made using the default conversions coded in the OZIPM4 MASS option. For VOC, that is a molecular weight of 14.5 grams per carbon atom and for NOX it is 46 grams per mole.

APPENDIX B

Example EKMA Inputs and Ouputs

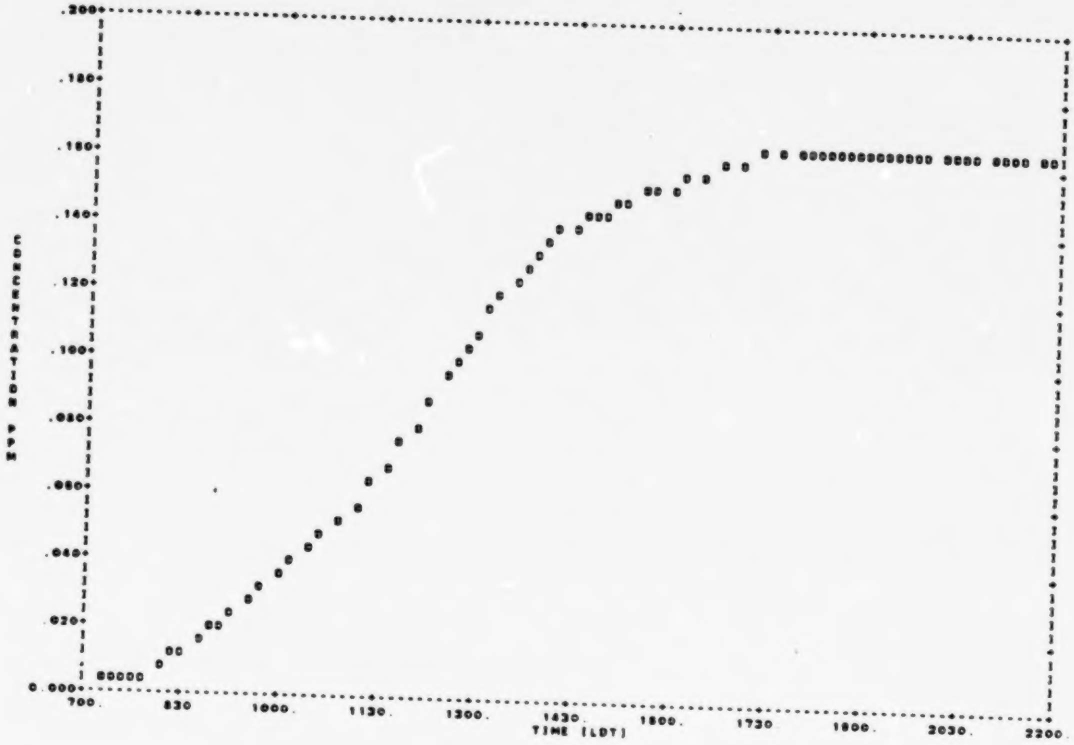
Information supplied by Chameides.............	Pages B-2 to B-5
Information produced as part of this study.....	Pages B-6 to B-8

```
PLACE     33.65     84.417    5.0       1984.     6.        04.
ATLANTA AIRPORT
TIME      700.      2200.
DILU      250.      1515.
SPEC      1.
03
TITL
 current conditions  ISOP = 30 kg/km2/day
MASS      -12.      .679      .096      250.      30.0
0.0       11.0184   4.9254    4.9254    4.2026    3.426     1.9446
.476      .6193     .7034     .7034     .7034
0.0       10.8496   4.556     4.556     3.4293    2.5576    1.462
.2332     .2848     .3711     .3711     .3711
ISOP      0.        1.        2.        3.        4.        5.
5.        5.        4.        3.        2.        1.
TRANS     0.0       .039      .038      .020      0.0       0.0
CALC      .679      .096

*
```

```
          *    OZONE ISOPLETH PLOTTING PACKAGE    *
          *       WITH OPTIONAL MECHANISMS        *
          *                                       *
          *              O Z I P M                *
          *                                       *
          *            VERSION 4.00               *
          *                                       *
          *          DECEMBER, 1987               *
          *                                       *


:HE INPUTS FOR THIS RUN ARE

       PLACE     33.85     84.417    5.0       1984.     6.        04.
       ATLANTA AIRPORT
       TIME      700       2200.
       DILU      250.      1515.
       SPEC      1.
       O3
       TITL
        current conditions  ISOP = 30 kg/km2/day
       MASS      -12.      .878      .085      250.      30.0
       0.0       11.0184   4.9254    4.9254    4.2025    3.425     1.8445
       .478      .8183     .7034     .7034     .7034
       0.0       10.8498   4.866     4.866     3.4283    2.8878    1.482
       .2332     .2848     .3711     .3711     .3711
       ISOP      0.        1.        2.        3.        4.        5.
       6.        5.        4.        3.        2.        1.
       TRANS     0.0       .038      .038      .020      0.0       0.0
       CALC      .878      .085
VOC  EMISSIONS:      .87800   .990008E-02
 0.000000   .109092   .048765   .048765   .041808   .033830   .018263   .004713   .008132   .008884   .008884   .008884
NOX  EMISSIONS:      .08600   .220468E-01
 0.000000   .239189   .100441   .100441   .075802   .058384   .032231   .008141   .008278   .008181   .008181   .008181
ISOP EMISSIONS:  35.00000      .0001   .11525E+03
 0.000000115.246098230.492197345.738295460.984394576.230492576.230492576.230492460.984394345.738295230.492197115.246098





                     current conditions  ISOP = 30 kg/km2/day

                    PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

                            ATLANTA AIRPORT

                    LATITUDE       33.850

                    LONGITUDE      84.417

                    TIME ZONE      5.0

                    DATE           6       4    1984

                    TIME           700     TO   2200      LOCAL DAYLIGHT TIME

                    DILUTION DETERMINED FROM THE FOLLOWING

                    INVERSION HEIGHTS      INITIAL   250.      FINAL      1515.

                    TIMING                 START     800.      STOP       1500.

                    MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

                    TIME        800     900     1000     1100     1200     1300     1400     1500

                    HEIGHT      250.0   250.0   474.2    784.0    1013.6   1204.5   1338.0   1437.8

                    REACTIVITY

                    EMISSIONS        ETH  FRACTION  .037   OLE  FRACTION  .035   ALD2 FRACTION  .052

                    EMISSIONS        FORM FRACTION  .021   TOL  FRACTION  .088   XYL  FRACTION  .117

                    EMISSIONS        PAR  FRACTION  .584   ISOP FRACTION 0.000   NR   FRACTION  .085

                    SURFACE LAYER    ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037

                    SURFACE LAYER    FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .028

                    SURFACE LAYER    PAR  FRACTION  .488   ISOP FRACTION 0.000   NR   FRACTION  .273

                    ALOFT            ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037

                    ALOFT            FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .028

                    ALOFT            PAR  FRACTION  .488   ISOP FRACTION 0.000   NR   FRACTION  .273

                    NO2/NOX          .250
```

```
TRANSPORTED CONCENTRATIONS

SURFACE LAYER        OZONE   0.000      HYDROCARBON   .039    NOX     0.000 PPM

ALOFT                OZONE    .039      HYDROCARBON   .020    NOX     0.000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR          1     2     3     4     5     6     7     8     9    10
                         11    12

  VOC     FRACTION    0.000  .109  .048  .045  .043  .034  .019  .005  .006  .007
                       .007  .007

  NOX     FRACTION    0.000  .239  .100  .100  .075  .056  .032  .005  .006  .006
                       .006  .006

  ISOP    FRACTION    0.000*****************************************************
                     ************
```

```
                                           current conditions  ISOP = 30 kg/km2/day

 TIME       NMOC        NMOC/          NOX          NO2         O3
(LDT )     TOTAL         NOX          TOTAL       FRACTION    (INSTANT)

  700.     .71704      7.46817        .09600       .25000      0.00000
                                                                  0.00000

  800.     .70700      7.48426        .09448       .30875       .00553
                                                                   .00787

  900.     .41118      6.92012        .05942       .54853       .01529
                                                                   .04591

 1000.     .28823      7.28170        .03954       .67371       .03565
                                                                   .13741

 1100.     .20286      8.14190        .02492       .74640       .05506
                                                                   .27141

 1200.     .16759     10.46620        .01601       .80624       .07820
                                                                   .46664

 1300.     .14185     17.72395        .00800       .88741       .10861
                                                                   .75356

 1400.     .12148     40.78771        .00298       .90622       .13507
                                                                  1.11183

 1500.     .10953     69.28785        .00158       .92253       .14564
                                                                  1.32646

 1600.     .10583     77.33745        .00137       .93111       .15451
                                                                  1.48287

 1700.     .10334     73.37906        .00141       .94096       .16053
                                                                  1.55447

 1800      .10254     65.35698        .00157       .95675       .16424
                                                                  1.60257

 1900      .10267     59.68052        .00172       .96731       .16533
                                                                  1.61036

 2000      .10180     77.14762        .00132       .99999       .16470
                                                                  1.61790

 2100      .10099    144.07429        .00070       .99999       .16367
                                                                  1.62064

 2200.     .10046    197.24716        .00051       .99999       .16267
                                                                  1.61869

                 MAXIMUM ONE HOUR AVE O3    =  .16528 CENTERED AT 1801. LDT
```



current conditions ISOP = 30 kg/km2/day

O3 CONCENTRATION AS A FUNCTION OF TIME

```
TITLE
ATLANTA WITH 30 KG/KM2 ISOP
PLACE     33.65      84.417     5.         1984.      6.         4.
ATLANTA
TIME      700.       2200.
DILU      250.       1515.
TRAN      0.0000     0.0390     0.0380     0.0200     0.0000     0.0000
MOLE      -12.0      3.0        250.       1000000.   0.679      0.096
.00001
VOC       0.0        757.3954   338.5678   338.5678   288.8831   235.5003
133.6701  32.71983   42.57015   48.35111   48.35111   48.35111
NOX       0.0        234.7864   98.59231   98.59231   74.21040   55.34672
31.63783  5.046472   6.163101   8.030642   8.030642   8.030642
ISOP      0.0        11.78385   23.56770   35.35156   47.13541   58.91927
58.91927  58.91927   47.13541   35.35156   23.56770   11.78385
CALC      0.679      0.096
```

```
ATLANTA WITH 30 KG/KM2 ISOP

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

       ATLANTA

LATITUDE    33.650

LONGITUDE   84.417

TIME ZONE   5.0

DATE        6    4   1984

TIME        700  TO  2200    LOCAL DAYLIGHT TIME

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS     INITIAL  250.    FINAL     1515.

TIMING                START    800.    STOP      1500.

MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME      800    900    1000    1100    1200    1300    1400    1500
HEIGHT    250.0  250.0  474.2   754.0  1013.8  1204.5  1339.0  1437.9

REACTIVITY
EMISSIONS       ETH  FRACTION  .037   OLE  FRACTION  .035   ALD2 FRACTION  .052
EMISSIONS       FORM FRACTION  .021   TOL  FRACTION  .089   XYL  FRACTION  .117
EMISSIONS       PAR  FRACTION  .564   ISOP FRACTION  .000   NR   FRACTION  .085
SURFACE LAYER   ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037
SURFACE LAYER   FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026
SURFACE LAYER   PAR  FRACTION  .498   ISOP FRACTION  .000   NR   FRACTION  .273
ALOFT           ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037
ALOFT           FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026
ALOFT           PAR  FRACTION  .498   ISOP FRACTION  .000   NR   FRACTION  .273
NO2/NOX        .250

TRANSPORTED CONCENTRATIONS

SURFACE LAYER        OZONE     .000      HYDROCARBON   .038    NOX       .000 PPM
```

```
ALOFT              OZONE    .039     HYDROCARBON   .020    NOX      .000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES    HOUR        1     2     3     4     5     6     7     8     9    10
                      11    12
  VOC     FRACTION   .000  .109  .049  .049  .042  .034  .019  .005  .006  .007
                     .007  .007
  NOX     FRACTION   .000  .239  .100  .100  .076  .056  .032  .005  .006  .008
                     .008  .008
  ISOP    FRACTION   .000########################################################
                    ############


                                 ATLANTA WITH 30 KG/KM2 ISOP
 TIME      NMOC       NMOC/       NOX        NO2        O3
 (LDT )    TOTAL       NOX       TOTAL     FRACTION  (INSTANT)
  700.    .71705     7.46927    .09600     .25000     .00000
  800.    .70703     7.48423    .09447     .30858     .00563
  900.    .41159     6.92803    .05941     .54646     .01929
 1000.    .26848     7.27752    .03689     .67371     .03686
 1100.    .20319     8.16186    .02490     .74641     .05506
 1200.    .16780    10.48941    .01600     .80814     .07820
 1300.    .14198    17.76196    .00799     .86744     .10861
 1400.    .12159    40.86810    .00298     .90823     .13506
 1500.    .10980    69.38779    .00158     .92262     .14562
 1600.    .10580    77.48268    .00137     .93109     .15448
 1700.    .10351    73.48405    .00141     .94092     .16059
 1800.    .10278    65.35793    .00157     .95871     .16424
 1900.    .10291    59.63336    .00173     .98729     .16524
 2000.    .10184    77.77531    .00131     .99999     .16459
 2100.    .10096   144.86530    .00070     .99999     .16356
 2200.    .10046   197.43950    .00051     .99999     .16257
                   MAXIMUM ONE HOUR AVE O3    =  .16518 CENTERED AT 1901. LDT
```

APPENDIX C

Revised EKMA Inputs Used in Sensitivity Tests

I. EKMA inputs for the case with no biogenic emissions:

```
TITLE
ATLANTA ASSUMING NO BIOGENIC EMISSIONS
PLACE    33.65     84.417    4.        1984.     6.        4.
ATLANTA
TIME     800.      1900.
DILU     250.      1515.
TRAN     0.0000    0.0390    0.0380    0.0200    0.0000    0.0000
MOLE     -11.0     2.0       250.      1000000.  0.679     0.096
VOC      757.3954  338.5678  338.5678  288.8831  235.5003  133.6701
32.71983 42.57015  48.35111  45.86963  40.91354
NOX      234.7864  98.59231  98.59231  74.21040  55.34672  31.63783
5.046472 6.163101  8.030642  7.229958  5.628590
CALC     0.679     0.096
EKMA     0.147     7.075
```

II. EKMA inputs for the case with total isoprene emissions of 30 kg/km^2:

```
TITLE
ATLANTA WITH 30 KG/KM2 ISOP
PLACE    33.65     84.417    4.        1984.     6.        4.
ATLANTA
TIME     800.      1900.
DILU     250.      1515.
TRAN     0.0000    0.0390    0.0380    0.0200    0.0000    0.0000
MOLE     -11.0     3.0       250.      1000000.  0.679     0.096
.00001
VOC      757.3954  338.5678  338.5678  288.8831  235.5003  133.6701
32.71983 42.57015  48.35111  45.86963  40.91354
NOX      234.7864  98.59231  98.59231  74.21040  55.34672  31.63783
5.046472 6.163101  8.030642  7.229958  5.628590
ISOP     11.78385  23.56770  35.35156  47.13541  58.91927  58.91927
58.91927 47.13541  35.35156  23.56770  11.78385
CALC     0.679     0.096
EKMA     0.147     7.075
```

APPENDIX D

EKMA Inputs for Other Exceedences

```
TITLE
ATL 4/26/86 DEKALB
PLACE     33.65     84.417    4.        1986.     4.        26.
ATLANTA
TIME      800.      1900.
DILU      250.      1515.
TRAN      0.0000    0.0540    0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.564     0.080
VOC       766.2284  799.7662  655.0978  340.8293  334.4915  349.3667
365.22486 414.6483  518.3963  460.0642  361.2104
NOX       248.7659  235.0742  184.0945  92.38160  90.16132  96.31144
329.25366 385.0217  555.4329  469.3578  323.4520
CALC      0.564     0.080
EKMA      0.142     7.075


TITLE
ATL 6/26/86 DEKALB
PLACE     33.65     84.417    4.        1986.     6.        26.
ATLANTA
TIME      800.      1900.
DILU      250.      1515.
TRAN      0.0000    0.0560    0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.546     0.075
VOC       766.2284  646.0311  338.5678  340.8293  334.4915  349.3667
365.22486 414.6483  518.3963  460.0642  361.2104
NOX       248.7659  189.5802  91.28877  92.38160  90.16132  96.31144
329.25366 385.0217  555.4329  469.3578  323.4520
CALC      0.546     0.075
EKMA      0.163     7.075


TITLE
ATL 6/27/86 DEKALB
PLACE     33.65     84.417    4.        1986.     6.        27.
ATLANTA
TIME      800.      1900.
DILU      250.      1515.
TRAN      0.0000    0.0620    0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.488     0.078
VOC       766.2284  646.0311  338.5678  340.8293  334.4915  349.3667
365.22486 414.6483  518.3963  460.0642  361.2104
NOX       248.7659  189.5802  91.28877  92.38160  90.16132  96.31144
329.25366 385.0217  555.4329  469.3578  323.4520
CALC      0.488     0.078
EKMA      0.160     7.075
```

```
TITLE
ATL 7/18/86 DEKALB
PLACE     33.65     84.417    4.        1986.     7.        18.
ATLANTA
TIME      800.      1900.
DILU      250.      1515.
TRAN      0.0000    0.0580    0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.716     0.118
VOC       766.2284  799.7662  655.0978  340.8293  334.4915  349.3667
365.22486 414.6483  518.3963  460.0642  361.2104
NOX       248.7659  235.0742  184.0945  92.38160  90.16132  96.31144
329.25366 385.0217  555.4329  469.3578  323.4520
CALC      0.716     0.118
EKMA      0.164     7.075


TITLE
ATL 7/23/86 DEKALB
PLACE     33.65     84.417    4.        1986.     7.        23.
ATLANTA
TIME      800.      1900.
DILU      250.      1515.
TRAN      0.0000    0.0680    0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.710     0.093
VOC       766.2284  799.7662  655.0978  340.8293  334.4915  349.3667
365.22486 414.6483  518.3963  460.0642  361.2104
NOX       248.7659  235.0742  184.0945  92.38160  90.16132  96.31144
329.25366 385.0217  555.4329  469.3578  323.4520
CALC      0.710     0.093
EKMA      0.164     7.075


TITLE
ATL 7/31/86 DEKALB
PLACE     33.65     84.417    4.        1986.     7.        31.
ATLANTA
TIME      800.      1800.
DILU      250.      1287.
TRAN      0.0000    0.051     0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.524     0.075
VOC       766.2284  646.0311  338.5678  340.8293  334.4915  349.3667
365.22486 414.6483  518.3963  460.0642  361.2104
NOX       248.7659  189.5802  91.28877  92.38160  90.16132  96.31144
329.25366 385.0217  555.4329  469.3578  323.4520
CALC      0.524     0.075
EKMA      0.152     7.075
```

```
TITLE
ATL 7/10/84 CONYERS
PLACE     33.65     84.417    4.        1984.     7.        10.
ATLANTA
TIME      800.      1900.
DILU      250.      1515.
TRAN      0.0000    0.039     0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.644     0.091
VOC       757.39547 338.56781 338.56781 340.82933 284.89939 243.43970
251.53717 152.46343 41.154130 45.869636 40.913543
NOX       234.78646 98.592311 98.592311 92.381601 76.000043 59.010398
189.70098 127.80284 24.622364 22.865750 17.879053
CALC      0.644     0.091
EKMA      0.155     7.075


TITLE
ATL 8/22/84 CONYERS
PLACE     33.65     84.417    4.        1984.     8.        22.
ATLANTA
TIME      800.      1900.
DILU      250.      1287.
TRAN      0.0000    0.043     0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.540     0.052
VOC       757.3954  338.5678  338.5678  288.8831  235.5003  133.6701
32.719836 42.57015  48.35111  45.86963  40.91354
NOX       234.7864  98.59231  98.59231  74.21040  55.34672  31.63783
16.029970 19.57691  25.50909  22.96575  17.87805
CALC      0.540     0.052
EKMA      0.147     7.075


TITLE
ATL 6/26/85 CONYERS
PLACE     33.65     84.417    4.        1985.     6.        26.
ATLANTA
TIME      800.      1900.
DILU      250.      2465.
TRAN      0.0000    0.046     0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  1.672     0.236
VOC       757.3954  338.5678  287.7558  236.9369  128.9615  32.15617
40.913543 42.57015  48.35111  45.86963  40.91354
NOX       234.7864  98.59231  73.66507  56.03921  29.57336  4.866859
17.879053 19.57691  25.50909  22.96575  17.87805
CALC      1.672     0.236
EKMA      0.145     7.075
```

```
TITLE
ATL 7/12/85 CONYERS
PLACE     33.65     84.417    4.        1985.     7.        12.
ATLANTA
TIME      800.      1900.
DILU      250.      1287.
TRAN      0.0000    0.037     0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.512     0.072
VOC       757.3954  338.5678  338.5678  288.8831  235.5003
32.719836 42.57015  48.35111  45.86963  40.91354
NOX       234.7864  98.59231  98.59231  74.21040  55.34672  31.63783
16.028970 18.57691  25.50909  22.96575  17.87905
CALC      0.512     0.072
EKMA      0.145     7.075
```

```
TITLE
ATL 6/26/86 CONYERS
PLACE     33.65     84.417    4.        1986.     6.        26.
ATLANTA
TIME      800.      1900.
DILU      250.      1287.
TRAN      0.0000    0.056     0.0380    0.0200    0.0000    0.0000
MOLE      -11.0     2.0       250.      1000000.  0.546     0.075
VOC       757.3954  338.5678  338.5678  340.8293  284.9993  243.4397
138.02821 34.59641  48.35111  45.86963  40.91354
NOX       234.7864  98.59231  98.59231  92.38160  76.00004  59.01039
106.84437 17.84091  25.50909  22.96575  17.87905
CALC      0.546     0.075
EKMA      0.165     7.075
```

APPENDIX C

Final Report

URBAN AIRSHED MODEL STUDY OF FIVE CITIES

Low-Cost Application of the Model to Atlanta and Evaluation of the Effects of Biogenic Emissions on Emission Control Strategies

SYSAPP-89/117

15 September 1989

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1 INTRODUCTION

The job of reducing ozone concentrations to levels below the National Ambient Air Quality Standard (NAAQS) has proven to be far more difficult than was thought when the Clean Air Act was passed and amended. The level of ozone precursor emissions remains too high; either emission reductions have been too small or have been required of the wrong sources, or both.

A plethora of technical explanations has been offered for failure to attain the ozone standard. These include perceived weaknesses in the attainment planning process (Federal Registrar, Vol. 52, No. 226, November 24, 1987; OTA 1988a,b,c), incomplete understanding or recognition of the anthropogenic and natural factors that cause elevated tropospheric ozone levels (Science, 1988), the failure to consider the effects of natural emissions (Chameides et al., 1988; Morris et al., 1989), use of a simplistic modeling approach (OTA, 1988a; Seinfeld, 1988a; Burton, 1988), and failure to reduce the amount of emissions intended, either through overestimates of the effectiveness of control technology or failure to account for certain categories of emission sources. The EPA, after lengthy consideration, has proposed a comprehensive policy that includes major changes in the planning process for reducing ozone concentrations (Federal Registrar, Vol. 52, No. 226, November 24, 1987). These changes include improvements in modeling practices and requirements for improving the data to support improved modeling practices. The EPA is now evaluating public comments on the proposed policy.

USE OF THE URBAN AIRSHED MODEL

The EPA recommends that states use the Urban Airshed Model (UAM) for the modeling of ozone and photochemical reactive pollutants in urban areas (EPA, 1986). An alternative approach, the Empirical Kinectics Modeling Approach (EKMA), has been accepted for demonstrating attainment of the ozone standard in most State Implementation Plans (Federal Registrar, Vol. 52, No. 226, 1987). The UAM and EKMA are quite different types of models; the UAM is a three-dimensional grid model while the EKMA is a trajectory box model.

A reluctance to use the UAM in the past is based on the perception that it requires using data from costly intensive measurement studies and requires extensive computational resources. Most of the cost of applying the UAM is attributed to the practice of conducting an extensive evaluation of UAM performance, which usually entails many diagnostic simulations. This evaluation enables us to understand why the UAM performs as it does for a particular application and, if deemed necessary, to take actions to improve model performance. Historically, it has been expected that the UAM will calculate hourly ozone concentrations to within approximately 15 to 20 percent of the observed peak value (Seinfeld, 1988a; Burton, 1988). More recent applications of the UAM to the Los Angeles basin have used routinely available meteorological data and predicted observed ozone levels with a high degree of skill (Seinfeld, 1988a; Burton, 1988; Hogo, Mahoney, and Yocke 1988). A recent application of the UAM to the New York metropolitan area used simple inputs, i.e., constant wind fields and mixing depths (Rao 1987).

This simplified use of the UAM, relying on routinely available data and reducing the requirement for strict evaluations of model performance, offers air quality managers a practical air quality assessment tool for identifying emission control strategies that demonstrate attainment of the ozone NAAQS. This simplified approach is called Practice-for-Low-Cost-Airshed-Application-for-Nonattainment-Regions (PLANR). The PLANR use of the UAM requires almost the same quantity and quality of inputs as EKMA, and the overall application cost is substantially reduced. The possible exception is the emissions inventory, which in PLANR applications should contain the same spatially (horizontally and vertically) and temporally varying emissions used in standard UAM applications (such detail is necessary to account for the differing reactivities of VOC emissions). However, local agencies generally have emissions inventories at hand; in addition, UAM input inventories can be readily estimated from existing national emissions inventories (e.g., the National Acid Precipitation Program 1980 and 1985 inventories). Knowledge of current emission rates is needed to estimate the emission controls required to achieve attainment of the ozone NAAQS.

The PLANR use of the UAM may not be appropriate for all nonattainment regions. When attainment is expected to be imminent, improved methods for using EKMA may be adequate. In other, more complex situations, such as the Los Angeles basin, the Houston region, and the New York Metropolitan area among others, the complexity of meteorological conditions and the emissions distribution and the severity of the ozone attainment problem probably require a more detailed application of the UAM. The application of UAM to these more complex situations, called Practice-of-Airshed-Application-in-Complex-Regions (PACR), would involve more extensive model performance requirements and hence more diagnostic simulations, and a resultant increase in costs. However, even for a complex nonattainment region, the PLANR approach would probably be more comprehensive and reliable than EKMA for estimating the controls needed to achieve ozone attainment.

THE "FIVE CITIES" UAM STUDY

The EPA has funded a study of the PLANR approach in five urban areas in the U.S. (New York, St. Louis, Atlanta, Philadelphia, and Dallas-Ft. Worth). The main objectives of this "Five Cities" study are to:

(1) Demonstrate the usefulness of PLANR for air quality planning;

(2) Determine the effects of alternative fuels and alternative Reid vapor pressure values for fuels on urban ozone concentrations;

(3) Demonstrate the use of PLANR to evaluate SIP control strategies and compare results with those obtained with EKMA; and

(4) Transfer the UAM model, modeling data bases, and applications technology to the states for use in future SIPs.

In addition, the study includes two city-specific analyses:

(1) For the St. Louis and Philadelphia areas, comparison of the PLANR use of the UAM (i.e., using only routinely available data) with applications of the UAM that use an extensive data base; and

(2) The effects of biogenic emissions on anthropogenic emission reductions in the Atlanta area.

Previous reports on the "Five Cities" study have documented the PLANR use of UAM and the evaluation of alternative fuel emission scenarios for the New York metropolitan area and the city of St. Louis (Morris et al., 1989a). This report presents the PLANR use of the UAM for Atlanta and analyzes the effects of biogenic emissions on the anthropogenic VOC emission reductions required to meet attainment of the ozone NAAQS. Recently, the EKMA model was applied to Atlanta for 4 June 1984 to estimate the effects of biogenic emissions on VOC emission controls needed to bring Atlanta into attainment of the ozone NAAQS (Chameides et al., 1988). One of the purposes of this study is to repeat this analysis using a more comprehensive model, the UAM(CB-IV).

2 DESCRIPTION OF THE CB-IV VERSION OF THE URBAN AIRSHED MODEL

The Urban Airshed Model (UAM) is a three-dimensional grid model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the various physical and chemical processes that take place in the atmosphere. The basis of the UAM is the atmospheric diffusion or species continuity equation. This equation represents a mass balance in which all of the relevant emissions, transport, diffusion, chemical reaction, and removal processes are expressed in mathematical terms. Based on the grid concept, the model is generally employed to simulate an 8- to 72-hour period during which episodic meteorological conditions persist.

Because the model can resolve both spatial and temporal features of the concentration field, it is well suited to the analysis of future control strategies and their effects on air quality in various parts of the modeling region. Before the model is used for such an analysis, its ability to replicate measurements from an historical ozone episode is tested. Model inputs are prepared from observed meteorological, emission, and air quality data for a particular day or days. Once the model inputs have been adjusted within the range of their uncertainty so that the model performs within prescribed levels, the emission inventory can be changed to represent assumptions about future emission scenarios. The model is then re-run with the forecasted emissions, and the resulting hourly ozone patterns are what the model predicts is likely to occur under meteorological conditions similar to the historical episode.

The UAM is the only air quality model recommended by the EPA for photochemical or reactive pollutant modeling applications involving entire urban areas (EPA, 1986). The EPA guidelines refer to the 1978-1980 version of the UAM; the formulation of that version is discussed by Ames and others (1985a,b). Many improvements to the UAM have been made over the last 10 years. The two most significant are:

Incorporation of the latest version of the Carbon-Bond Mechanism, the CB-IV (Gery, Whitten, and Killus, 1988)

Use of the Smolarkiewicz algorithm for advection (Smolarkiewicz, 1983)

USE OF THE SMOLARKIEWICZ ALGORITHM TO SOLVE THE ADVECTION EQUATION

Grid-based air quality simulation models require a numerical approximation of the horizontal advection terms in the species conservation equations. The 1978-1980 version of the Urban Airshed Model (UAM) used a variant of the Sharp and Smooth Transport Algorithm (SHASTA) originally formulated by Boris and Book (1973). Since 1977 there have been many comparative studies of advection schemes. Examples of such studies relevant to the UAM are those of Zalesak (1970), Schere (1983), Chock and Dunker (1983), Chock (1985), Smolarkiewicz (1983), and Yamertino and Scire (1985). In each of these studies an idealized scalar function (a cone, block, ellipse, or cosine wave) representative of a concentration distribution is advected by a rotating wind field (constant angular velocity). The rotating wind field provides a range of Courant numbers, depending on the radial distance from the center of the domain. The degree to which the attributes of the idealized function (total mass, peak value, mean value, and gradients) are preserved indicates the accuracy of the scheme.

The above studies showed that a number of advection schemes were more accurate than SHASTA, as measured by the idealized tests. For the UAM, a number of specific requirements constrained the selection of alternative to SHASTA. First, it is important that the scheme be positive definite, i.e., that it not result in negative concentrations. Second, the scheme should use forward time differencing to minimize storage requirements and to insure compatibility with the chemical mechanism numerical solution scheme. Third, the ability of an advection scheme to represent the magnitudes and locations of peak concentrations is of major importance in regulatory applications. Fourth, to handle complex airflows, the scheme should display relatively uniform accuracy over a wide range of Courant numbers (i.e., wind speeds).

Further review indicated that the advection scheme developed by Smolarkiewicz (1983) represented the best combination of accuracy and economy. The Smolarkiewicz scheme is conceptually similar to SHASTA in that a highly diffusive transport step is followed by an anti-diffusive correction step. The transport step is essentially the well-known "upstream" finite-difference scheme. The correction step involves a second exercise of the upstream finite difference scheme, substituting the anti-diffusive velocity for the actual velocity. The Smolarkiewicz scheme is positive definite and forward in time, and can be used in either a time-split or multidimensional mode. Smolarkiewicz demonstrated that the scheme was superior in both accuracy and economy to the multidimensional generalization of SHASTA formulated by Zalesak (1979). In applications to the Los Angeles area and Kern County, California, the UAM with the Smolarkiewicz algorithm produced results that were more accurate than those produced in earlier applications using SHASTA (Hogo, Mahoney, and Yocke, 1988; Whitten et al., 1985).

USE OF THE CB-IV TO SOLVE PHOTOCHEMISTRY

The latest version of the Carbon-Bond Mechanism (CBM-IV) was recently implemented in the UAM (Gery, Whitten, and Killus, 1988). Whenever a new chemical kinetics mechanisms is merged into a complex air quality simulation model, the predictive capabilities and solution speed of the new computer code require optimization and evaluation. This process is even more important now because the recent gas-phase chemical kinetics mechanisms (CAL, RADM, and the CBM-IV) are larger than previous mechanisms, and therefore require significantly more computing time. The CBM-IV reactions are shown in Table 1. There are some minor differences between the original CB-IV and the version implemented in the UAM. For the examination of ethanol (ETOH) blended fuels, ETOH was added as a species. The ethanol reaction is $ETOH + OH \rightarrow ALD2 + HO_2$ with a rate constant of 4,300 1/ppm-min. Both numerical and chemical improvements were made to the CB-IV implementation in the UAM so that computational speed could be increased and solution uncertainty diminished.

TABLE 1. The Carbon Bond Mechanism-IV.*

Number	Reaction[1]	Reaction Rate Data Pre-factor (ppm^{-n}min^{-1})	 Temp. Factor exp((-E/R)/T)	 Rate Constant @ 298K k_{298} (ppm^{-n}min^{-1})
1)	NO2 -hν1-> NO + O			see notes
2)	O -----> O3	8.383 E+04	*EXP(1175/T)	4.323 E+06
3)	O3 + NO -----> NO2	2.643 E+03	*EXP(- 1370/T)	2.664 E+01
4)	O + NO2 -----> NO	1.375 E+04		1.375 E+04
5)	O + NO2 -----> NO3	2.303 E+02	*EXP(687/T)	2.309 E+03
6)	O + NO -----> NO2	3.233 E+02	*EXP(602/T)	2.438 E+03
7)	O3 + NO2 -----> NO3	1.760 E+02	*EXP(- 2450/T)	4.731 E-02
8)	O3 -hν1-> O	5.300 E-02		5.300 E-02×k_1
9)	O3 -hν4-> O1D			see notes
10)	O1D -----> O	1.147 E+05	*EXP(390/T)	4.246 E+05
11)	O1D + H2O -----> 2.00OH	3.260		3.260
12)	O3 + OH -----> HO2	2.344 E+03	*EXP(- 940/T)	1.000 E+02
13)	O3 + HO2 -----> OH	2.100 E+01	*EXP(- 580/T)	2.999
14)	NO3 -hν1-> 0.89NO2 + 0.89O + 0.11NO	3.390 E+01		3.390 E+01×k_1
15)	NO3 + NO -----> 2.00NO2	1.909 E+04	*EXP(250/T)	4.416 E+04
16)	NO3 + NO2 -----> NO + NO2	3.660 E+01	*EXP(- 1230/T)	5.901 E-01
17)	NO3 + NO2 -----> N2O5	7.849 E+02	*EXP(256/T)	1.853 E+03
18)	N2O5 + H2O -----> 2.00HNO3	1.900 E-06		1.900 E-06
19)	N2O5 -----> NO3 + NO2	2.110 E+16	*EXP(-10897/T)	2.776
20)	NO + NO -----> 2.00NO2	2.600 E-05	*EXP(530/T)	1.539 E-04
21)	NO + NO2 + H2O -----> 2.00HONO	1.600 E-11		1.600 E-11
22)	OH + NO -----> HONO	6.554 E+02	*EXP(806/T)	9.799 E+03
23)	HONO -hν1-> OH + NO	1.975 E-01		1.975 E-01×k_1
24)	OH + HONO -----> NO2	9.770 E+03		9.770 E+03
25)	HONO + HONO -----> NO + NO2	1.500 E-05		1.500 E-05
26)	OH + NO2 -----> HNO3	1.537 E+03	*EXP(713/T)	1.682 E+04
27)	OH + HNO3 -----> NO3	7.600	*EXP(1000/T)	2.179 E+02
28)	HO2 + NO -----> OH + NO2	5.482 E+03	*EXP(240/T)	1.227 E+04
29)	HO2 + NO2 -----> PNA	1.640 E+02	*EXP(749/T)	2.025 E+03
30)	PNA -----> HO2 + NO2	2.876 E+15	*EXP(-10121/T)	5.115
31)	OH + PNA -----> NO2	1.909 E+03	*EXP(380/T)	6.833 E+03
32)	HO2 + HO2 -----> H2O2	8.739 E+01	*EXP(1150/T)	4.144 E+03
33)	HO2 + HO2 + H2O -----> H2O2	7.690 E-10	*EXP(5800/T)	2.181 E-01
34)	H2O2 -hν3-> 2.00OH	2.550 E-01		2.550 E-01×k_{39}
35)	OH + H2O2 -----> HO2	4.720 E+03	*EXP(- 187/T)	2.520 E+03
36)	OH + CO -----> HO2	3.220 E+02		3.220 E+02
37)	FORM + OH -----> HO2 + CO	1.500 E+04		1.500 E+04
38)	FORM -hν2-> CO + 2.00HO2			see notes
39)	FORM -hν3-> CO			see notes
40)	FORM + O -----> OH + HO2 + CO	4.302 E+04	*EXP(- 1550/T)	2.370 E+02
41)	FORM + NO3 -----> HNO3 + HO2 + CO	9.300 E-01		9.300 E-01
42)	ALD2 + O -----> C2O3 + OH	1.739 E+04	*EXP(- 986/T)	6.360 E+02
43)	ALD2 + OH -----> C2O3	1.037 E+04	*EXP(250/T)	2.400 E+04
44)	ALD2 + NO3 -----> C2O3 + HNO3	3.700		3.700
45)	ALD2 -hν6-> FORM + XO2 + CO + 2.00HO2			see notes
46)	C2O3 + NO -----> NO2 + XO2 + FORM + HO2	7.915 E+03	*EXP(250/T)	1.831 E+04
47)	C2O3 + NO2 -----> PAN	1.180 E-04	*EXP(5500/T)	1.223 E+04
48)	PAN -----> C2O3 + NO2	5.616 E+18	*EXP(-14000/T)	2.220 E-02
49)	C2O3 + C2O3 -----> 2.00FORM + 2.00XO2 + 2.00HO2	3.700 E+03		3.700 E+03
50)	C2O3 + HO2 -----> 0.79FORM + 0.79XO2 + 0.79HO2 + 0.79OH	9.600 E+03		9.600 E+03
51)	OH -----> XO2 + FORM + HO2	6.521 E+03	*EXP(- 1710/T)	2.100 E+01

(Continued)

* As currently implemented in the UAM (CB-IV), ethanol and methanol have been added to the CB-IV and can be treated as explicit species.

TABLE 1. Concluded.

Number	Reaction[1]			Reaction Rate Data	
			Pre-factor (ppm^{-n}min^{-1})	Temp. Factor exp((-E/R)/T)	Rate Constant @ 298K k_{298} (ppm^{-n}min^{-1})
52)	PAR + OH	----->	0.87XO2 + 0.13XO2N + 0.11HO2 + 0.11ALD2 + 0.76ROR - 0.11PAR	1.203 E+03		1.203 E+03
53)	ROR	----->	1.10ALD2 + 0.96XO2 + 0.94HO2 + 0.04XO2N + 0.02ROR - 2.10PAR	6.250 E+16	*EXP(- 8000/T)	1.371 E+05
54)	ROR	----->	HO2	9.545 E+04		9.545 E+04
55)	ROR + NO2	----->		2.200 E+04		2.200 E+04
56)	O + OLE	----->	0.63ALD2 + 0.38HO2 + 0.28XO2 + 0.30CO + 0.20FORM + 0.02XO2N + 0.22PAR + 0.20OH	1.756 E+04	*EXP(- 324/T)	5.920 E+03
57)	OH + OLE	----->	FORM + ALD2 + XO2 + HO2 - PAR	7.740 E+03	*EXP(504/T)	4.200 E+04
58)	O3 + OLE	----->	0.50ALD2 + 0.74FORM + 0.33CO + 0.44HO2 + 0.22XO2 + 0.10OH - PAR	2.104 E+01	*EXP(- 2105/T)	1.800 E-02
59)	NO3 + OLE	----->	0.91XO2 + FORM + ALD2 + 0.09XO2N + NO2 - PAR	1.135 E+01		1.135 E+01
60)	O + ETH	----->	FORM + 0.70XO2 + CO + 1.70HO2 + 0.30OH	1.540 E+04	*EXP(- 792/T)	1.080 E+03
61)	OH + ETH	----->	XO2 + 1.56FORM + HO2 + 0.22ALD2	3.000 E+03	*EXP(411/T)	1.192 E+04
62)	O3 + ETH	----->	FORM + 0.42CO + 0.12HO2	1.856 E+01	*EXP(- 2633/T)	2.700 E-03
63)	OH + TOL	----->	0.08XO2 + 0.36CRES + 0.44HO2 + 0.56TO2	3.106 E+03	*EXP(322/T)	9.150 E+03
64)	TO2 + NO	----->	0.90NO2 + 0.90HO2 + 0.90OPEN	1.200 E+04		1.200 E+04
65)	TO2	----->	CRES + HO2	2.500 E+02		2.500 E+02
66)	OH + CRES	----->	0.40CRO + 0.60XO2 + 0.60HO2 + 0.30OPEN	6.100 E+04		6.100 E+04
67)	CRES + NO3	----->	CRO + HNO3	3.250 E+04		3.250 E+04
68)	CRO + NO2	----->		2.000 E+04		2.000 E+04
69)	OPEN	-hν->	C2O3 + HO2 + CO	9.040		9.040 $\times k_{38}$
70)	OPEN + OH	----->	XO2 + 2.00CO + 2.00HO2 + C2O3 + FORM	4.400 E+04		4.400 E+04
71)	OPEN + O3	----->	0.03ALD2 + 0.62C2O3 + 0.70FORM + 0.03XO2 + 0.69CO + 0.08OH + 0.76HO2 + 0.20MGLY	8.030 E-02	*EXP(- 500/T)	1.500 E-02
72)	OH + XYL	----->	0.70HO2 + 0.50XO2 + 0.20CRES + 0.80MGLY + 1.10PAR + 0.30TO2	2.453 E+04	*EXP(116/T)	3.620 E+04
73)	OH + MGLY	----->	XO2 + C2O3	2.600 E+04		2.600 E+04
74)	MGLY	-hν->	C2O3 + HO2 + CO	9.640		9.640 $\times k_{38}$
75)	O + ISOP	----->	0.60HO2 + 0.80ALD2 + 0.55OLE + 0.50XO2 + 0.50CO + 0.45ETH + 0.90PAR	2.700 E+04		2.700 E+04
76)	OH + ISOP	----->	XO2 + FORM + 0.67HO2 + 0.40MGLY + 0.20C2O3 + 1.00ETH + 0.20ALD2 + 0.13XO2N	1.420 E+05		1.420 E+05
77)	O3 + ISOP	----->	FORM + 0.40ALD2 + 0.55ETH + 0.20MGLY + 0.10PAR + 0.06CO + 0.44HO2 + 0.10OH	1.800 E-02		1.800 E-02
78)	NO3 + ISOP	----->	XO2N	4.700 E+02		4.700 E+02
79)	XO2 + NO	----->	NO2	1.200 E+04		1.200 E+04
80)	XO2 + XO2	----->		2.550 E+01	*EXP(1300/T)	2.000 E+03
81)	XO2N + NO	----->		1.000 E+03		1.000 E+03

The implementation of the CB-IV in the UAM used a modified Crank-Nicholson algorithm for the simultaneous solution of the differential equations that represent the chemical changes for each species. This numerical integration scheme produced results that were within a few percent of those obtained with the previous (Gear) algorithm over a wide range of atmospheric conditions (Morris et al., 1989a,c).

3 MODELING EPISODE AND DOMAIN SELECTION

EPISODE SELECTION

Table 2 lists all days from the years 1984 to 1987 in Georgia (either Atlanta or Columbus) in which the maximum daily ozone concentration at any monitor in the AIRS data base exceeds the National Ambient Air Quality Standard of 120 ppb. Of the 62 days where ozone concentrations in Georgia are greater than or equal to 120 ppb, 61 pertain to Atlanta and one (3/18/84) to Columbus (note that on other days Columbus may have an exceedence of the ozone standard but the ozone concentrations are less than recorded in Atlanta). The most striking feature of the occurrence of elevated ozone concentrations in Atlanta are the months of July and August, 1987, where in a 21 day period (19 July to 7 August 1987) there were 15 exceedences of ozone NAAQS. This period also included the very highest observed ozone concentration in Atlanta (201 ppb on 31 July 1987). On most days during this period, most ozone monitors in Georgia, including Columbus, are recording high ozone concentrations. This seems to indicate a region wide buildup of ozone concentrations over an extended length of time and area. Thus, the elevated ozone concentrations in Atlanta during July and August, 1987, may be attributable to regional-scale in addition to urban-scale ozone formation.

For Atlanta, the city specific analysis will analyze the effects of biogenic emissions on urban ozone formation and on the effects of anthropogenic VOC emissions strategies designed to reduce ozone. A previous study on the effects of biogenic emissions for Atlanta used the EKMA model to analyze ozone formation on 4 June 1984. It is highly desirable that this day also be chosen for the city-specific UAM analysis as long as there are no other specific reasons, such as excessive wind shear or other unusual meteorological phenomena, that would preclude its selection. On 4 June 1984, the maximum daily ozone concentration was 147 at Conyers, Georgia. For the two day period of 3 to 4 June 1984, winds are predominantly from the

TABLE 2. Highest ozone days in Atlanta, 1984 - 1987.

Rank	Peak 03	Monitor	Date	Maximum Daily Ozone 130890002 Panthers. DKLB	130970002 Sweetwat. SWTR	131210053 MLK MLKM	132150008 Columbus COLO	132470001 Conyers CNYR
1	201.	130890002	7/31/87	201.	98.	141.	118.	163
2	169.	130890002	8/ 1/87	169.	130.	138.	80.	158.
3	168.	130970002	7/24/87	140.	168.	155.	113.	90.
4	165.	132470001	6/26/86	163.	-99.	-99.	95.	165.
5	164.	130890002	7/18/86	164.	-99.	-99.	90.	142.
6	164.	130890002	7/23/86	164.	-99.	-99.	92.	111.
7	160.	130890002	6/27/86	160.	-99.	-99.	67.	131.
8	157.	132470001	8/ 2/87	138.	88.	128.	70.	157.
9	155.	132470001	7/10/84	115.	-99.	-99.	53.	155.
10	155.	130970002	7/23/87	154.	155.	153.	100.	85.
11	155.	130970002	7/25/87	113.	155.	118.	90.	94.
12	152.	132150008	3/18/84	60.	-99.	-99.	152.	-99.
13	151.	130890002	7/31/86	151.	-99.	-99.	108.	114.
14	150.	132470001	6/ 9/87	129.	73.	103.	75.	150.
15	150.	130970002	7/30/87	112.	150.	113.	93.	93.
16	149.	131210053	7/26/87	129.	100.	149.	98.	88.
17	147.	132470001	6/ 4/84	130.	-99.	-99.	83.	147.
18	147.	132470001	8/22/84	118.	-99.	-99.	78.	147.
19	146.	130890002	8/ 3/87	146.	118.	128.	80.	129.
20	145.	132470001	6/26/85	115.	-99.	-99.	72.	145.
21	145.	132470001	7/12/85	118.	-99.	-99.	65.	145.
22	144.	132470001	6/10/87	137.	95.	115.	85.	144.
23	142.	130890002	4/26/86	142.	-99.	-99.	100.	105.
24	140.	130970002	8/21/87	99.	140.	104.	68.	98.
25	140.	132470001	6/16/86	118.	-99.	-99.	108.	140.
26	137.	130890002	7/22/86	137.	-99.	-99.	80.	84.
27	137.	132470001	8/ 2/86	112.	-99.	-99.	103.	137.
28	136.	130890002	8/ 4/87	136.	100.	113.	75.	116.
29	136.	130890002	8/ 5/87	136.	95.	103.	100.	120.
30	136.	130890002	6/28/84	136.	-99.	-99.	55.	122.
31	135.	130890002	6/ 6/85	135.	-99.	-99.	67.	127.
32	135.	130890002	7/29/87	135.	128.	118.	88.	132.
33	133.	130970002	6/11/87	103.	133.	103.	120.	86.
34	133.	130970002	9/ 3/87	91.	133.	95.	78.	80.
35	133.	132470001	9/14/84	105.	-99.	-99.	103.	133.
36	132.	132470001	6/ 2/87	109.	68.	86.	63.	132
37	132.	132470001	9/ 2/87	108.	88.	89.	90.	132.
38	131.	132470001	8/ 1/86	114.	-99.	-99.	85.	131.
39	131.	130890002	5/13/85	131.	-99.	-99.	83.	72.
40	130.	132470001	6/ 4/85	120.	-99.	-99.	-99.	130.
41	130.	130890002	6/24/87	130.	75.	104.	53.	118.
42	130.	132150008	7/27/87	108.	108.	94.	130.	120.
43	130.	132470001	8/ 7/87	129.	78.	107.	63.	130.
44	129.	132470001	8/ 4/86	114.	-99.	-99.	103.	129
45	129.	130890002	7/19/86	129.	-99.	-99.	90.	112.
46	128.	132470001	6/ 3/87	103.	65.	72.	75.	128.
47	127.	130890002	8/18/84	127.	-99.	-99.	83.	100.
48	127.	132470001	6/ 5/85	92.	-99.	-99.	67.	127.
49	126.	130890002	7/19/87	126.	115.	109.	73.	75.
50	125.	132470001	8/23/87	115.	78.	96.	83.	125.
51	125.	132470001	6/ 1/84	97.	-99.	-99.	75.	125.
52	125.	132470001	6/ 3/84	105.	-99.	-99.	70.	125.
53	125.	132470001	7/11/85	118.	-99.	-99.	63.	125.
54	125.	130890002	7/ 8/86	125.	-99.	-99.	60.	123.
55	123.	130890002	8/16/86	123.	-99.	-99.	78.	93.
56	123.	130890002	7/21/86	123.	-99.	-99.	90.	110.
57	122.	132470001	7/20/85	115.	-99.	-99.	83.	122.
58	122.	132470001	8/ 1/85	95.	-99.	-99.	85.	122.
59	122.	130890002	7/26/86	122.	-99.	-99.	78.	74.
60	121.	130890002	6/22/86	121.	-99.	-99.	78.	85.
61	120.	130890002	7/22/87	120.	98.	116.	68.	82.
62	120.	130970002	8/20/87	100.	120.	108.	75.	96.

northwest sector with some southwesterlies late on 4 June. Maximum daily ozone concentrations on 4 June are 78 ppb (DLLS) upwind of Atlanta and 130 (DKLB) and 147 (CNYR) ppb at distances of, respectively, 15 and 40 km downwind of Atlanta (see Figure 1). Thus, it appears that there is not a large amount of transported ozone into the Atlanta region on 4 June 1984 and the ozone exceedence is predominantly due to emissions from the Atlanta area.

Since the 4 June 1984 ozone event is not overly influenced by transported ozone and, as will be shown in the next section, does not contain any unusual meteorological conditions it appears to be an appropriate day for the city-specific biogenic analysis for Atlanta and a demonstration of the PLANR use of the UAM. Since it is desirable to minimize the effects of initial conditions in any UAM simulation, the UAM modeling episode will be initialized on 3 June 1984 and terminated the evening of 4 June 1984. Thus, UAM modeling inputs will be prepared for 3 and 4 June 1984 with the actual starting time on 3 June to be determined from an inert tracer simulation.

It should be noted that other days listed in Table 2 may be more appropriate for demonstrating ozone attainment in a State Implementation Plan (SIP). Generally, it would be desirable for a SIP to pick a day with a higher ozone concentration, a day closer in time to current, a day in which the elevated ozone concentrations can be attributed to Atlanta, and a day that represents typical meteorological conditions that produces ozone exceedences in Atlanta. The very highest ozone concentration in Table 1 (201 ppb observed on 31 July 1987) appears to be an anomalous event since it is almost 20 percent higher than any of the other high ozone events over the four year period.

MODELING DOMAIN SELECTION

The modeling domain for the 3 - 4 June 1984 UAM modeling episode should include a fairly large fetch upwind of the city of Atlanta in order to account for sufficient amounts of biogenic emissions upwind of the urban core of Atlanta. The modeling domain should also include enough area downwind of Atlanta in order to capture the maximum ozone concentrations that will be formed. Grid spacing should be sufficiently small in order to resolve the anthropogenic emission distribution in

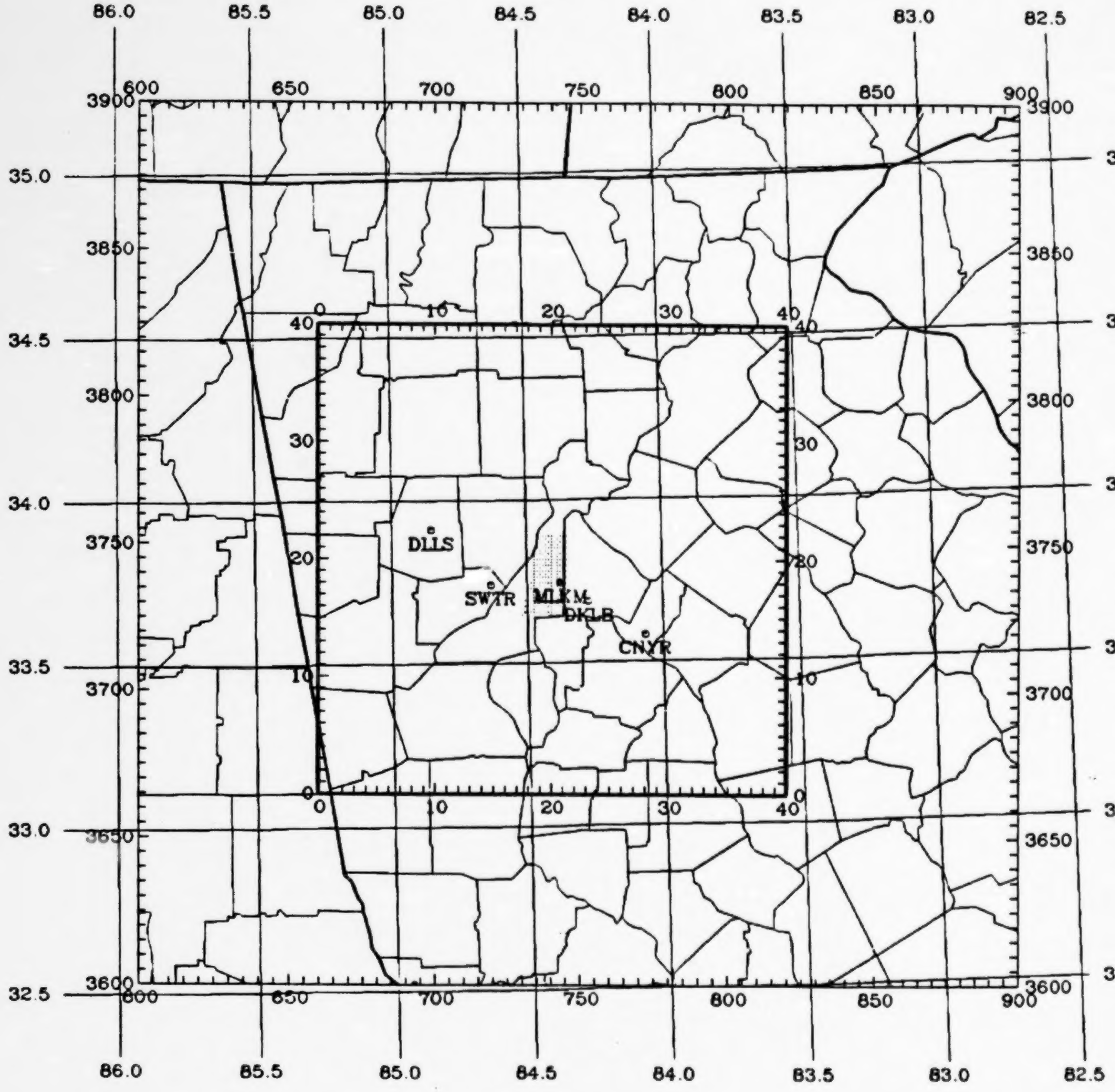

86.0
85.5
85.0
84.5
84.0
83.5
83.0
82.5
600
650
700
750
800
850
900
3900
3850
3800
3750
3700
3650
3600
35.0
34.5
34.0
33.5
33.0
32.5
0
10
20
30
40
DLLS
SWTR
MLKM
DKLB
CNYR

Figure 1. UAM modeling domain for Atlanta. Modeling domain consists of 40 by 40 array of 4 km grid cells with an origin at UTM coordinates 660 km easting, 3665 km northing, zone 16.

Atlanta. To determine the UAM modeling domain synoptic weather maps along with upper-air data from Athens and Waycross, Georgia; Nashville, Tennessee; and Centreville-Brent, Alabama, and surface data from South Dekalb were analyzed to determine the mean flow conditions that existed on 3-4 June 1984.

Meteorological Conditions on 3-4 June 1984

The days of 3 and 4 June 1984 saw the passage of a high pressure system. The 500 mb height contours at 0700 EST on 4 June 1984 shows the approaching high pressure ridge towards Atlanta. The 500 mb high pressure ridge passed through the region during the evening of the 4th of June. The axis of the surface high pressure system passed through the modeling region during the afternoon of the 4th. On the 3rd of June, daytime low level winds (<600m) were from the west at 3-6 ms^{-1} throughout the modeling region while aloft the winds were in the same direction, but stronger. As the axis of the high pressure system moved near the modeling region, a slight easterly component to the wind field developed (a result of the circulation about the high pressure system). This flow was first seen in the upper levels (> 600m) on the morning of the 4th, but by mid morning was seen in the surface layer. After the passage of the high pressure system, the winds became southwesterly. The weather conditions during the modeling period were clear, hot and humid. Maximum temperatures were in the upper 80's and dew point temperatures in the low 60's.

Modeling Domain Definition

Figure 1 gives a region-wide perspective of the modeling domain for Atlanta. As pictured in Figure 1, this modeling domain consists of a 40 by 40 array of 4 km square grid cells. The proposed modeling domain origin is located at UTM coordinates 660 km easting, 3665 km northing in zone 16 and extends 160 km in the east and north direction. As stated in the Atlanta UAM modeling protocol (SAI, 1988) 5 vertical layer structure is to be used in the UAM: two below the mixing height and three above. The region top will be based on the maximum mixing height occurring during the modeling episode.

In order to accommodate the city-specific analysis of the effects of biogenic emissions on urban ozone formation in Atlanta, there is a region 75 to 100 km wide upwind of Atlanta. This will allow for a 4 to 12 hour loading of biogenic emissions into the atmosphere upwind from the outskirts of Atlanta.

4 PREPARATION OF MODEL INPUTS

An important requirement of the PLANR use of the UAM is that the procedures used to prepare model inputs should be consistent with traditional applications of the model. Procedures to be followed in preparing UAM inputs with limited data availability must be flexible and clearly stated. When there is a lack of data, there must be recommended procedures to be used. However, flexibility is an important component of the construction of UAM inputs when limited data are available. These procedures are currently being refined and evaluated to determine the optimum methodologies for generating UAM inputs with limited data availability.

The preprocessor programs supplied with the 1978-1980 version of the UAM generally rely on an intensive measurement program; data are interpolated from these measurements to obtain gridded fields of input parameters required by the UAM. Over the last 10 years, many of these programs have become outdated. More recent applications of the UAM have prepared input files using only routinely available (although fairly dense) meteorological and air quality data (Hogo, Mahoney, and Yocke, 1988). However, the procedures used for input preparation have been developed on a case-by-case basis and are tailored to data availability. In this section we discuss the initial application of the PLANR procedures for preparing meteorological, air quality, and terrain inputs for the UAM in which UAM modeling inputs are prepared using only routinely available data.

ROUTINE DATA AVAILABLE FOR ATLANTA

On June 3 and 4, 1984 there were six surface meteorological observation sites operating in and around the city of Atlanta. Table 3 lists the six surface sites along with the locations and meteorological variables available at each site. There were no upper-air observation sites located within the UAM modeling domain. Thus, we made

TABLE 3. Surface meteorological observation sites, locations, and variables in the Atlanta region.

Site Name	Location UTM (Zone 16) UTMX	UTMY	Variables Measured
Atlanta Hartsfield International Airport	739.580	3726.148	WS, WD, T, T_D, P
Dobbins Naval Air Station	729.590	3755.498	WS, WD, T, T_D, P
Fulton County (Charlie Brown) Airport	729.947	3740.709	WS, WD, T, T_D
Dekalb Peachtree Airport	749.724	3752.306	WS, WD, T, T_D
Conyers Monastery Monitor	772.248	3719.869	WS, WD
South Dekalb Panthersville Monitor	752.780	3730.991	WS, WD, T, T_D

use of upper-air observations from five sites that surround the UAM modeling domain for generating wind and mixing height inputs. These five upper-air sites, their locations, and the distance to the city of Atlanta are given in Table 4. The closest upper-air site to Atlanta is Athens Georgia, approximately 100 km to the east-northeast. Air quality data in and around Atlanta during June, 1984 consisted of three monitoring sites as listed in Table 5. There were no air quality data available near the boundaries of the modeling domain for use in prescribing boundary conditions.

PREPARATION OF UAM INPUT FILES

The following paragraphs describe how the UAM input files were prepared for the PLANR application of the UAM to Atlanta.

DIFFBREAK

This file contains the daytime mixing height or nighttime inversion height for each column of cells at the beginning and end of each hour of the simulation. Hourly mixing heights were estimated at several surface meteorological sites through use of the hourly surface measurements of temperature and the twice daily upper-air observations from a representative upper-air site. The Athens Georgia upper-air site was felt to be most representative of upper-air conditions in Atlanta because its proximity to Atlanta. For three of the surface meteorological observation sites that recorded temperature (Fulton County Airport, Dobbins Air Force Base, and South Dekalb monitor) the diurnal variations in mixing heights were calculated using the RAMMET meteorological processor. These hourly values were then input into the standard UAM mixing height interpolation program, DFSNBK (Ames et al., 1985b) using the 1/r interpolation option to produce the hourly spatially varying fields of mixing heights. The maximum daily mixing height varied from approximately 1200 to 1350 meters above ground across the region. Two of the surface observations sites that recorded temperature were not used in the generation of the DIFFBREAK file; one (Dekalb Peachtree Airport) had missing temperature data for 4 June 1984 and data from the other site (Atlanta Hartsfield International Airport) were not available in time to perform the mixing height analysis.

TABLE 4. Upper-air observation sites, locations, and distance from Atlanta used in this study.

Site Name	Location Lat	 Long	UTM Coordinates (Zone 16) UTMX	 UTMY	Distance from Atlanta (km)
Athens, GA	35° 57'	83° 19'	839.644	3763.429	109
Nashville, TN	36° 15'	86° 34'	538.182	4012.482	199
Greensboro, NC	36° 5'	79° 57'	1134.426	4016.946	491
Waycross, GA	31° 15'	82° 24'	937.394	3467.152	328
Centerville-Brent, AL	32° 54'	87° 15'	475.841	3640.638	275

TABLE 5. Ozone monitor names and locations.

Monitor JD	Monitor Name	UTM Location (Zone 16) UTMX	 UTMY	Years Available (1984 - 1987)
130890002	DeKalb Jr. College (DKLB)	752.78	3730.99	1984 - 1987
130970002	Sweetwater Creek State Park (SWTR)	719.28	3736.10	1987
131210053	MLK Marta Station (MLKM)	743.10	3737.15	1987
132150008	Columbus Airport (COLO)	693.15	3799.91	1984 - 1987
132470001	Conyers Monastery (CNYR)	772.25	3719.87	1984 - 1987

REGIONTOP

This file contains the height of each column of cells at the beginning and end of each hour of the simulation. If this height is greater than the mixing height, the cell or cells above the mixing height are assumed to be within an inversion. For the application of the UAM(CB-IV) to Atlanta a constant 1,400 m AGL region top was used. This value was picked because it is 50 m above the maximum mixing height; thus all five vertical layers of the UAM are contained within the well mixed layer, offering the maximum vertical resolution possible with the five-layer UAM configuration.

WIND

This file contains the x and y components of the wind velocity for every grid cell for each hour of the simulation. There are two steps in creating the wind fields for Atlanta: (1) application of the Diagnostic Wind Model (DWM) (Morris et al., 1988, 1989a; Douglas and Kessler, 1988) using 15 vertical levels and data from the six surface and five upper-air meteorological observation sites; and (2) vertical interpolation of the 15-layer hourly wind fields into the five-layer UAM configuration used for the Atlanta application (see Morris et al., 1989a).

The DWM creates an hourly 15-layer wind field by first creating a wind field by adjusting a domain-mean wind (based on upper-air observations) for terrain effects (kinematic effects, thermodynamically generated slope flows, blocking, and deflection). Then the observational information is added to the wind field by weighting the initial wind field heavily away from the observations and the observed winds heavily in the vicinity of the observations.

The 15-layer wind fields created by the DWM are then vertically averaged into the UAM five layer configuration. Since the surface observations provide a more detailed representation of the air flows in the vicinity of Atlanta and their presence is only felt within the lowest layer of the DWM, the first UAM vertical layer was assumed to have the same wind field as the first DWM layer. The DWM first layer is also weighted 50 percent in the second UAM vertical layer. The wind fields for the remainder of the UAM vertical layers were obtained from the DWM wind fields using weighted averaging. The resultant five-layer wind field was then modified using the procedure suggested by O'Brien (1970), which minimizes the vertical velocity out of the top of the region. In this manner, the boundary concentration assumed to exist above the region top (TOPCONC) does not greatly influence concentrations within the modeling domain.

For the application of the UAM to Atlanta, three separate wind fields were created corresponding to evaluation runs number 1 and 2 and a sensitivity test reported in Appendix G. As will be discussed later in the section on the evaluation of the UAM, these wind fields were created using the procedures described above but differed in definition of the domain-mean wind and the surface observation sites used.

METSCALARS

This file contains the hourly values of the meteorological parameters that do not vary spatially. These scalars are the NO_2 photolysis rate constant, the concentration of water vapor, the temperature gradient above and below the inversion base, the atmospheric pressure, and the exposure class. The NO_2 photolysis rates were calculated for the CB-IV mechanism using procedures described by Schere and Demerjian (1977) and actinic flux data collected by Bass and co-workers (1980) (see Gery, Whitten, and Killus, 1988). The concentration of water was based on measurements of temperature and dewpoint at three of the surface meteorological observation sites. These three values were averaged to obtain the hourly input for the UAM. Water concentrations ranged from approximately 14,000 to 18,000 ppm. An atmospheric pressure value of 1 atmosphere was used.

Exposure class is a measure of near surface stability: +3 during high solar intensity to -2 at night with no clouds. Exposure class was assigned based on the solar intensity: a value of 2 at night and daytime values of either 0 (one hour day/night transition period) to 3. The temperature gradients below (TGRADBELOW) and above (TGRADABOVE) the inversion were based on the twice-daily upper-air soundings taken at Athens, Georgia, and hourly surface temperatures observed at Charlie

Brown Airport. Values for TGRADBELOW from the surface to the mixing height (approximately 1300 m AGL) from the Athens evening sounding (1900 LST) are -0.0096, -0.0103, and -0.0107 K/m for June 2 through 4, respectively. Based on these measurements, values for TGRADBELOW were -0.0105 K/m for exposure classes 2 and 3, -0.01 K/m for exposure class 1, and -0.098 for exposure class 0.

The Athens morning sounding (0700 LST) measured values for TGRADBELOW of 0.018 and 0.030 K/m on June 3 and 4 respectively, assuming a mechanical mixing height of 250 m AGL. Observed temperatures at 250 m on 3 and 4 June were, respectively, 295.6 and 297.8 K. Nighttime hourly values for TGRADBELOW were then calculated for June 3 and 4 based on the surface temperature at the Charlie Brown Airport and the measured value at 250 m from the 0700 LST sounding.

For predawn hours, the temperature gradient from 250 m to the region top (1,400 m) from the 0700 sounding at Athens was used, resulting in values for TGRADABOVE of -0.0025 and -0.0075 °K/m for June 3 and 4, respectively. For daytime hours a temperature at the mixing height was calculated for each hour of the day using the surface measurement at the Charlie Brown Airport and the value for TGRADBELOW. Then the hourly temperature gradient between the mixing height and the region top was estimated using the calculated value at the mixing height and the measured temperature from the 0700 sounding at Athens at 1,400 m AGL (290.8 and 290.7 K on June 3 and 4, respectively)

AIRQUALITY

This file contains the initial concentrations of each species for each grid cell at the start of the simulation. Since the UAM was initiated at 12 noon on June 3, 1984, most of the material from the initial conditions were advected out of the region by the morning of 4 June; thus, initial concentrations do not influence ozone formation on 4 June. Accordingly, initial concentrations were assigned to "clean values" as follows:

VOC	25 ppbc (using EKMA default speciation)
ISOP	0.001 ppb
NO_x	1 ppb (split 3/4 NO_2, 1/4 NO)
O_3	40 ppb
CO	200 ppb

BOUNDARY

This file contains the location of the modeling region boundaries. It also contains the concentration of each species that is used as the boundary condition along each boundary segment at each vertical level. For the application of the UAM to Atlanta, the minimum of a one-cell buffer of unsimulated cells was used (i.e. the boundary conditions), resulting in a simulation region of 152 km by 152 km. As will be discussed in the section on the evaluation of the UAM, two sets of boundary conditions were derived for evaluation runs number 1 and 2. For evaluation run number 1, "clean" values (listed previously) were specified for boundary conditions. However, these clean values may underestimate background concentrations because of the biogenic emissions which increase background VOC and ISOP (isoprene) concentrations above the clean background level. Thus in order to determine a better estimate of background conditions, a UAM simulation was carried out with no anthropogenic emissions (i.e., biogenic emissions and clean boundary concentrations only). During the day, isoprene and VOC concentrations ranged from approximately 0.5 to 2.0 ppb and 35 to 75 ppbC, respectively. Thus for the second evaluation simulation, a 1 ppb ISOP boundary condition was prescribed and VOC boundary conditions were set at 40 ppbC, where the increase from the clean value of 25 ppb was mainly (92%) due to the lower reactive PAR species and the remainder of the increase was due to increases in OLE. Boundary conditions for ozone (40 ppb) and NO_x (1 ppb) were the same as used in evaluation run 1.

TOPCONC

This file contains the concentration of each species for the area above the modeling region. Since the wind fields are processed to eliminate the vertical velocity through the region top, the model results are not sensitive to TOPCONC. Accordingly, the clean concentration values listed previously were used.

TEMPERATUR

This file contains the hourly temperature for each surface layer grid cell. Hourly spatial varying temperatures were obtained by using 1/r interpolation from the surface meteorological observations.

EMISSIONS

This file contains the ground-level emissions of NO, NO_2, CB-IV VOC species categories, and CO for each grid square for each hour of the simulation. Anthropogenic emission estimates were obtained from the 1985 NAPAP county-wide emissions inventory through a several step process which includes updating mobile source emissions from MOBILE-3 to MOBILE-4 based emission factors, applying summer weekday and episodic temperature adjustments, gridding of data using a known surrogate distribution, and speciation of the VOC and NO_x emissions into the CB-IV mechanism species.

The NAPAP motor vehicle emission categories were split into exhaust and evaporative emissions based on splitting factors using the MOBILE-3 emissions program and the same average temperature as was used in generating the NAPAP inventory. The MOBILE-4 emissions program was then exercised for the episodic temperature conditions on 4 June 1984 to obtain episodic evaporative and exhaust emissions. Estimate of running loss emissions (which are not included in the NAPAP inventory) were then obtained by applying the ratio of the running loss to the exhaust emission factors from the MOBILE-4 to the mobile exhaust VOC emission rate.

The county-wide area source emissions were then mapped to the 40 by 40 4 km^2 modeling domain by assigning each area source Source Classification Code (SCC) category to a known surrogate distribution. Known surrogate distributions include:

agriculture, urban, rural, and water from the national Geographical Information Services land-use data base; population from the 1980 census; airports and limited access roadways based on digitizing the locations of airports and freeways from standard USGS maps; and spatial coverage based on the fractional coverage of each grid cell in each county. The gridded area source emissions were then adjusted to hourly emissions for a summer weekday and speciated into CB-IV species based on their SCC codes.

Estimates of biogenic VOC emissions were obtained from EPA's Atmospheric Research and Exposure Assessment Laboratory (EPA/AREAL) on a 1/4° longitude by 1/6° latitude grid for the entire Southeast. The EPA/AREAL had biogenic emission estimates for the entire Southeast for a two-week period during 1980. These emission estimates consider the effects of episodic temperature and solar intensity on the biogenic emission estimates. Based on analysis of surface temperatures, it was determined that 26 August 1980 provided the best match with episodic temperature and light intensity conditions of 4 June 1984. The biogenic emissions from the 1/4° by 1/6° grid were gridded onto the 4 km square grid cells used in the UAM modeling based on spatial covering of grid cells. The biogenic emissions from EPA/AREAL were already speciated into CB-IV species.

The final EMISSIONS file was obtained by merging the gridded NAPAP area source emissions with the low-level point sources and the biogenic emissions. The resultant anthropogenic and biogenic emission rates and their spatial distribution are given in Appendix A. Of particular note is that biogenic VOC emissions account for approximately 65 percent of the VOC emissions within the modeling domain.

PTSOURCE

This file contains the point source information, including the stack height, temperature and flow rate, the plume rise, the grid cell into which the emissions are emitted, and the emissions rates for NO, NO_2, CB-IV VOC categories, and CO for each point source for each hour. The 1985 NAPAP point source emissions file was separated into low-level and elevated points based on plume rise estimates. Those point sources whose plume rise was less than 25 m for typical atmospheric conditions were considered low-level sources and were merged with the EMISSIONS file after applying the summer weekday and diurnal emission profiles supplied as part of the NAPAP point source inventory.

Elevated point sources from the 1985 NAPAP point source file were adjusted to summer episodic conditions with diurnal variation using the adjustments given in the point source file. The emissions were then speciated into CB-IV species based on their SCC and SIC codes. The resultant data was run through the UAM point source preprocessor for input to the UAM. As shown in Appendix A, point source NO_x (including electrical utilities) emissions account for approximately 50 percent of the total NO_x emissions within the modeling domain.

TERRAIN

This file contains the value of the surface roughness and deposition factor for each grid square. Each 4 km^2 grid cell was assigned to a land-use category based on the digitization of a standard USGS map of the modeling region. The land-use categories were then converted to roughness lengths and vegetation factors according to data published by Argonne National Laboratory (see Morris et al., 1989a).

CHEMPARAM

This file contains information regarding the chemical species to be simulated, including reaction rate constants, upper and lower bounds, activation energy, and reference temperature. Reaction rate constants correspond to those given in the report documenting the CB-IV mechanism (Gery, Whitten, and Killus, 1988), except that reactions for methanol (MEOH) and ethanol (ETOH) have also been added to the mechanism (see Morris et al., 1989a).

SIMCONTROL

This file contains the simulation control information, such as the time of the simulation, file option information, default information, and information on integration and chemistry time steps.

5 DEVELOPMENT OF A PLANR BASE CASE FOR ATLANTA

One of the key components of the PLANR use of the UAM is a limitation on the number of diagnostic simulations used to arrive at a base case. This is achieved by relaxing the strict model performance standards expected of the UAM in the past. Although the goal is to achieve a statisfactory level of performance with as few diagnostic simulations as possible, the model must show some skill in predicting ozone observations in order to have confidence that the model will respond properly to changes in emissions.

The minimal performance goal in the past was to have the predicted regional maximum ozone concentration be within 30 percent and in the general location of the peak observed value. Model performance has been considered good if the predicted peak ozone is within 15 percent. Clearly, when model inputs are based only on sparse routine data, rather than intensively measured data as in the past, model performance cannot be expected to always be as good in the past. However, there should be some minimal expectations of model performance since incorrect characterization of base case ozone concentrations may lead to incorrect calculations of ozone reductions due to alternative emission inputs.

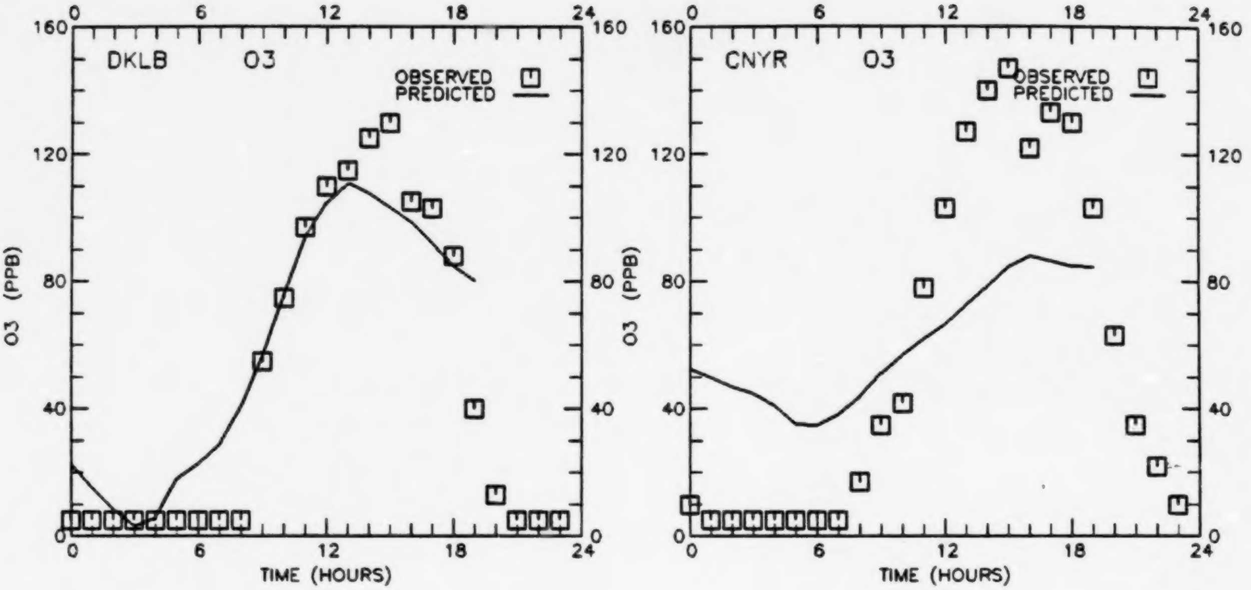
The protocols for several recent UAM studies of the impacts of California offshore drilling emissions (Haney et al., 1986; Yocke et al., 1985) defined a minimal model performance standard as follows: (1) the UAM-predicted regional maximum ozone concentration should be within 20 percent and in the general location of the observed maximum, and (2) the UAM predicted maximum at the location of the observed maximum should be within 30 percent of the observed value.

We adopted this model performance standard as a performance goal for the PLANR application of the UAM for Atlanta. However, model evaluation should always include discussions on whether the right answer is being obtained for the right reason. In addition, it may be useful to discuss approaches that may improve UAM performance but which also may deviate slightly from the demonstration of the PLANR use of the UAM. The PLANR use of the UAM for Atlanta discussed here involved three diagnostic simulations before an adequate base case was obtained that satisfied the minimal performance goal.

DIAGNOSTIC RUN 1

In the first diagnostic simulation, the UAM was exercised with clean boundary conditions (i.e., 40 ppb ozone, 25 ppbc VOC, 0.001 ppb ISOP, and 1 ppb NO_x), anthropogenic and biogenic emissions, and a first estimate of the wind field. The wind field was created using the DWM: the vertically varying domain-mean wind was defined as the vector average from the five upper-air soundings surrounding the modeling domain. The upper-air data obtained from the National Climatic Data Center (NCDC) on the TD9743 format was missing data from the lowest 1,500 m AGL of the 0700 June 4 upper-air sounding at Athens, Georgia. In addition, surface wind data was used from all of the surface sites, except Atlanta Hartsfield Airport, which was inadvertently left out of the initial analysis. Appendix B contains the wind fields generated by the DWM using the routine data from Atlanta and the procedures discussed above.

Hourly average predicted ozone concentrations for evaluation run 1 are contained in Appendix C. A comparison of predicted versus observed hourly ozone concentrations for the three monitors within the UAM modeling domain is given in Figure 2. As seen in Appendix C and Figure 2, the regional maximum predicted ozone concentration is 13.54 pphm, within 8 percent of the observed maximum of 14.7 at the Conyers Monastery (CNYR) ozone monitor. However, the predicted regional maximum is approximately 28 km (7 grid cells) to the north-north-west of the observed value. The maximum predicted ozone at the CNYR site for evaluation run 1 is 8.79 pphm, an approximate 40 percent underprediction of the observed maximum at that site. Model performance is better at the South Dekalb ozone monitor, where the maximum daily observed value of 13.0 pphm is reproduced to within 15 percent (11.1 pphm).



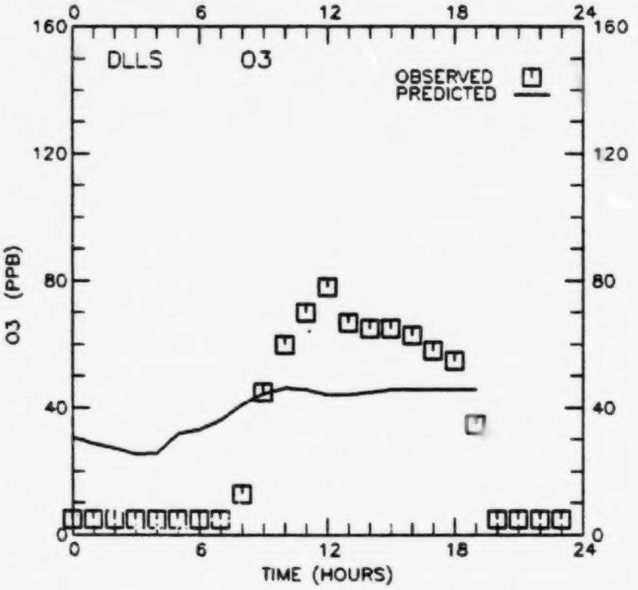


FIGURE 2. Observed and predicted ozone concentrations (ppb) for the Atlanta evaluation run 1.

However, concentrations are underpredicted at the Dallas (DLLS) ozone monitor, which lies upwind of the city of Atlanta. The maximum daily observed ozone concentration at DLLS of 7.8 pphm is underpredicted by about 60 percent (4.6 pphm).

DIAGNOSTIC RUN 2

Improvements Over Diagnostic Run 1

An analysis of the observed ozone features for 4 June 1984 indicates two major deviations of the predictions from the observations for diagnostic run 1: (1) the gross underprediction of the upwind monitor indicates that the ozone and ozone precursor loadings upwind of Atlanta are too low; and (2) the predicted cloud of elevated ozone concentrations appears to be too far north during the afternoon of 4 June 1984.

The fact that diagnostic run 1 is underpredicting the ozone at the upwind (DLLS) monitor is not surprising since clean background concentrations were used for the upwind boundary conditions. In particular, given the presence of biogenic VOC emissions in the area, the boundary VOC concentrations used in diagnostic run 1 (25 ppbc VOC; 0.001 ppb ISOP) are probably too low. In order to determine the magnitudes of VOC concentrations to use as boundary conditions, a UAM simulation without the anthropogenic emissions (i.e., biogenic emissions and clean boundary conditions only) was performed. This simulation of biogenic emissions only produced a maximum buildup of ISOP and VOC concentrations that ranged across the modeling domain from, respectively, 0.5 to 2.0 ppb and 35 to 75 ppbC. Thus we chose values a little lower than the midpoint of the maximum buildup, 1 ppb for ISOP and 40 ppbC for VOC, as boundary conditions in diagnostic run 2.

An examination of the observed ozone concentrations at the DLLS monitor on 4 June 1984 (see Figure 2) reveals that the observed maximum daily ozone concentration of 7.8 pphm occurs fairly early in the day (12 noon). This suggests that the peak observed ozone concentration at DLLS is mainly due to entrainment of ozone concentrations aloft as the mixing height rises rather than to local production of ozone due to local sources. Thus the boundary concentrations for ozone, and possibly NO_x, could justifiably be increased. However, we elected to keep the fairly low values for ozone and NO_x boundary conditions (40 and 1 ppb, respectively) for diagnostic run 2.

An examination of the observed winds, the predicted wind fields in diagnostic run 1 (Appendix B), and patterns of predicted hourly ozone concentrations (Appendix C) indicates that a southerly component in the wind field may occur too early in the afternoon. The persistence of a more northerly component in the winds in the late morning and early afternoon would result in the predicted cloud of elevated ozone concentrations impacting the CNYR monitor, producing a higher peak at that site. However, the wind measurements at the CNYR site observed southerly winds from about noon on. To determine whether this southerly wind was due to local effects or larger-scale flow features, the Georgia State meteorologist was consulted. The CNYR wind observation site is located near a grove of trees and may not be representative of mesoscale wind flows, and the Atlanta Hartsfield Airport wind observation site (which was inadvertently left out of the original analysis) was better sited (D. Kemmerick, personal communication, 1989). Thus, the CNYR wind measurement was eliminated and the Atlanta Hartsfield Airport winds added for the next evaluation run.

A new definition of the domain-mean wind was also used for the diagnostic run 2. Instead of a linear interpolation to the hour in question of a vector average of the five twice-daily upper-air soundings that surround Atlanta, most of which are over 200 km away, the Athens Georgia upper-air sounding alone was used to define the domain mean wind. Wind data for the lowest 1,500 m of the 4 June sounding at 1900 LST was supplied by the state of Georgia.

A further modification was made on the boundary definition of the diagnostic run 2. An examination of the spatial distribution of emissions (Appendix A) and the predicted hourly ozone concentrations from diagnostic run 1 (Appendix C) indicated that portions of the northern, southern, and western portions of the modeling domain could be eliminated without affecting the results. The boundary was thus modified and diagnostic run 1 was rerun to verify that the new boundary did not affect the computations.

Results of the Simulation

Diagnostic run 2 differed from run 1 in that (1) a higher VOC value was used (40 compared to 25 ppbC) and higher ISOP boundary conditions were used (1 compared to 0.001 ppb); (2) the domain-mean wind for the DWM came from the Athens upper-air sounding rather than a vector average from the five upper-air soundings; (3) the CNYR surface wind measurement was eliminated and the Atlanta Hartsfield wind measurement added to the analysis; (4) a minor mistake in the emissions inventory was corrected; and (5) the boundary was modified. The new UAM layer 1 wind fields generated for diagnostic run 2 are shown in Appendix D. The resulting predicted hourly ozone concentrations for evaluation run 2 are given in Appendix E. The predicted regional maximum ozone concentration is 13.2 pphm, within approximately 10 percent of the observed maximum. The predicted maximum ozone is approximately 22 km to the north of the observed maximum ozone. However, as shown in Figure 3, at the location of the peak observed ozone, the maximum observation is replicated to within less than 30 percent. In addition, the daily maximum observed ozone concentrations at the DKLB and DLLS monitor are reproduced to within, respectively, 18 and 36 percent.

Comparison of UAM grid cell-average concentrations with the point observations at the site of the observed ozone is a particularly stringent test. A slight incorrect characterization of the wind field, as is very likely when sparse data sets are used, will result in the placement of the elevated ozone plume away from the ozone monitor resulting in poor model performance statistics. However, this displacement of the ozone plume may not affect the model's response to emission control requirements. Thus it has been suggested that concentrations in adjacent grid cells (i.e., nearest neighbor) also be compared with the observed value in order to determine whether the ozone cloud is just slightly displaced (Seinfeld, 1988a; Burton, 1988). Figures 4 and 5 compare the observed and predicted hourly ozone concentrations resulting from a one-cell and two-cell search of the predicted concentrations closest to the observed values. At the CNYR monitor the predicted maximum daily ozone concentration for the point, a one-cell search, and a two-cell search matches the observed value of 14.7 pphm to within, respectively, 29, 25, and 22 percent. However, at the other two monitors (DKLB and DLLS), the nearest-neighbor analysis also

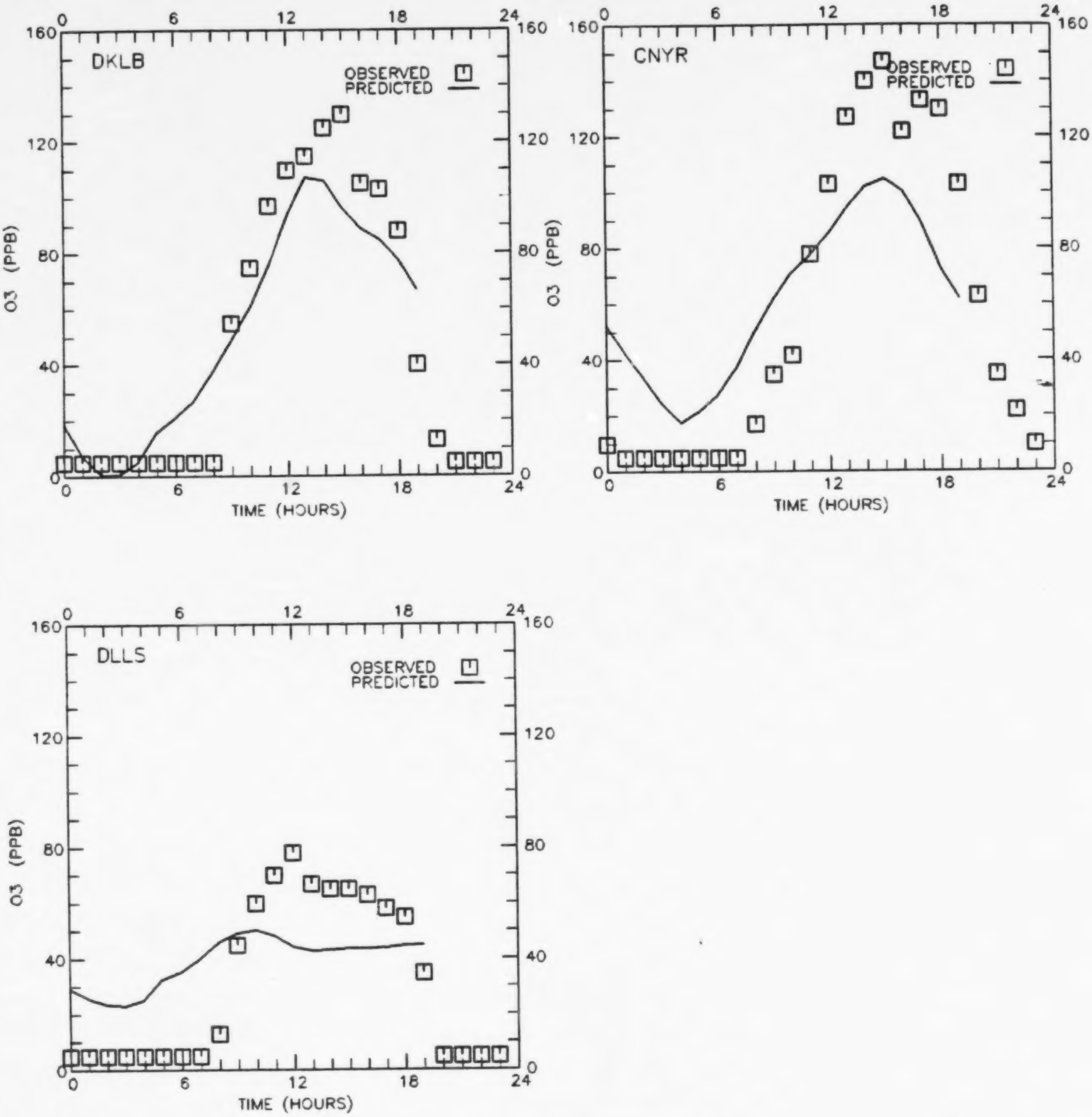


FIGURE 3. Observed and predicted ozone concentrations (ppb) for the Atlanta evaluation run 2.

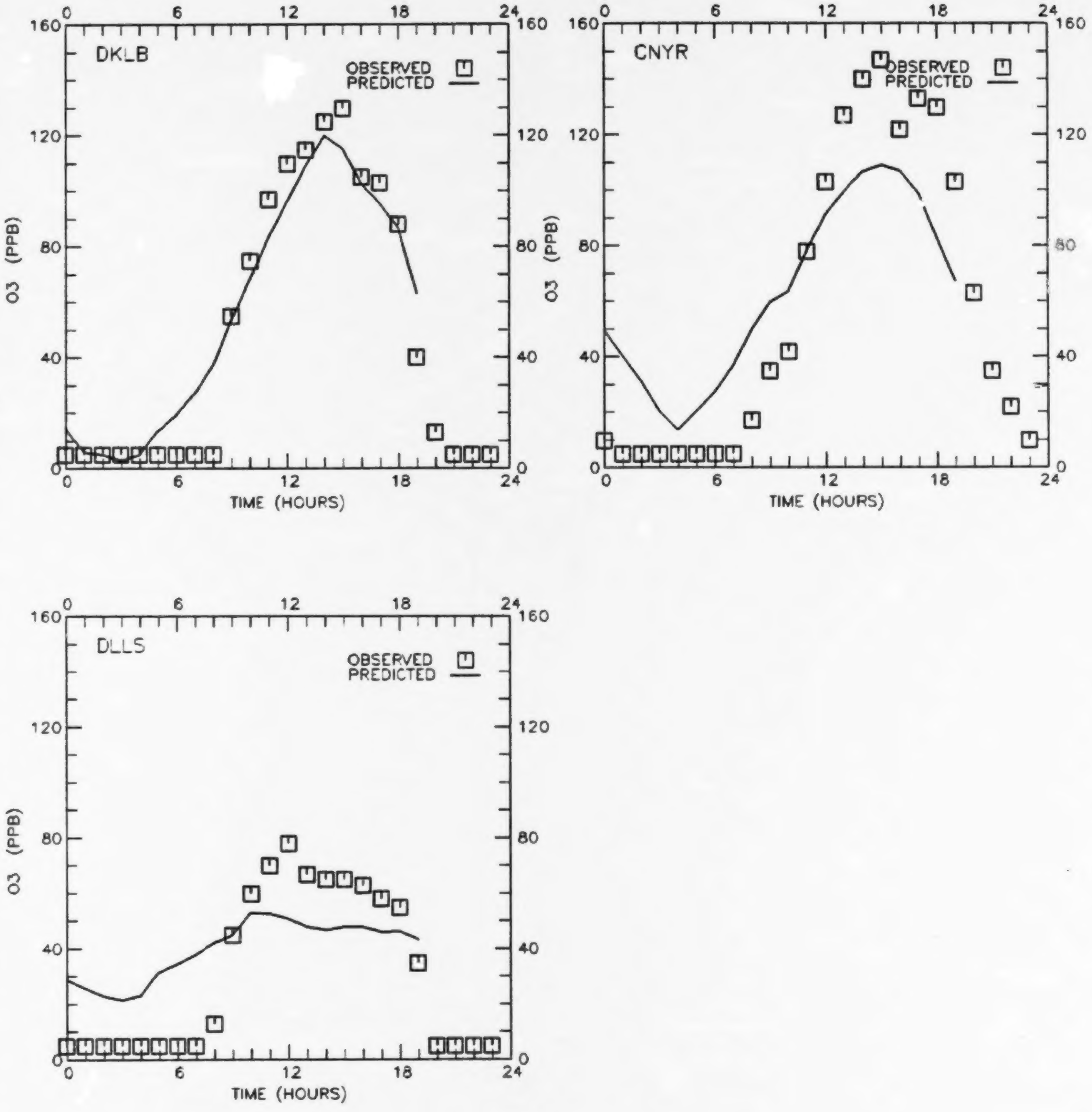


FIGURE 4. Observed and nearest-neighbor predicted (one-cell search) ozone concentrations (ppb) for the Atlanta evaluation run 2.

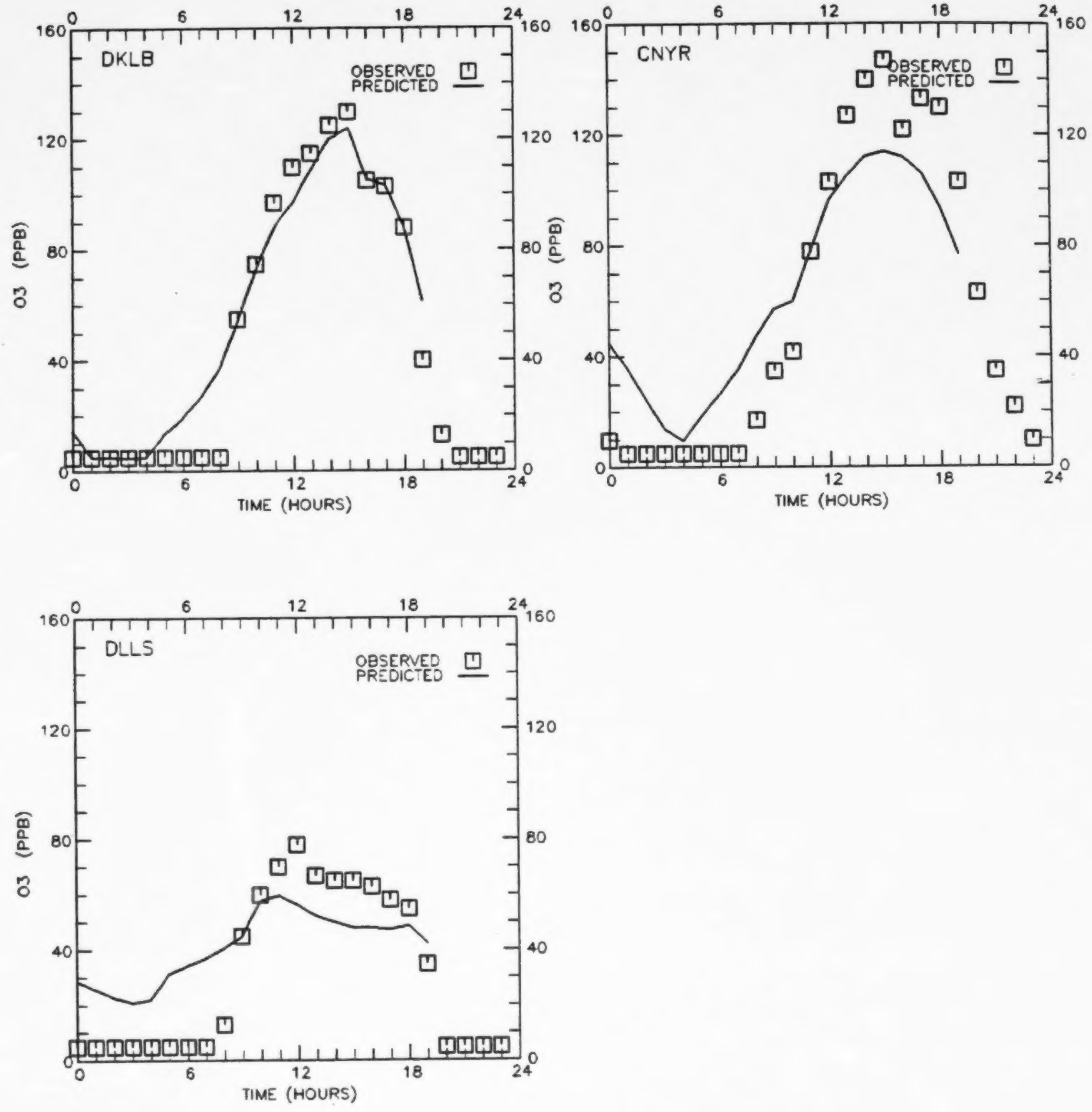


FIGURE 5. Observed and nearest-neighbor predicted (two-cell search) ozone concentrations (ppb) for the Atlanta evaluation run 2.

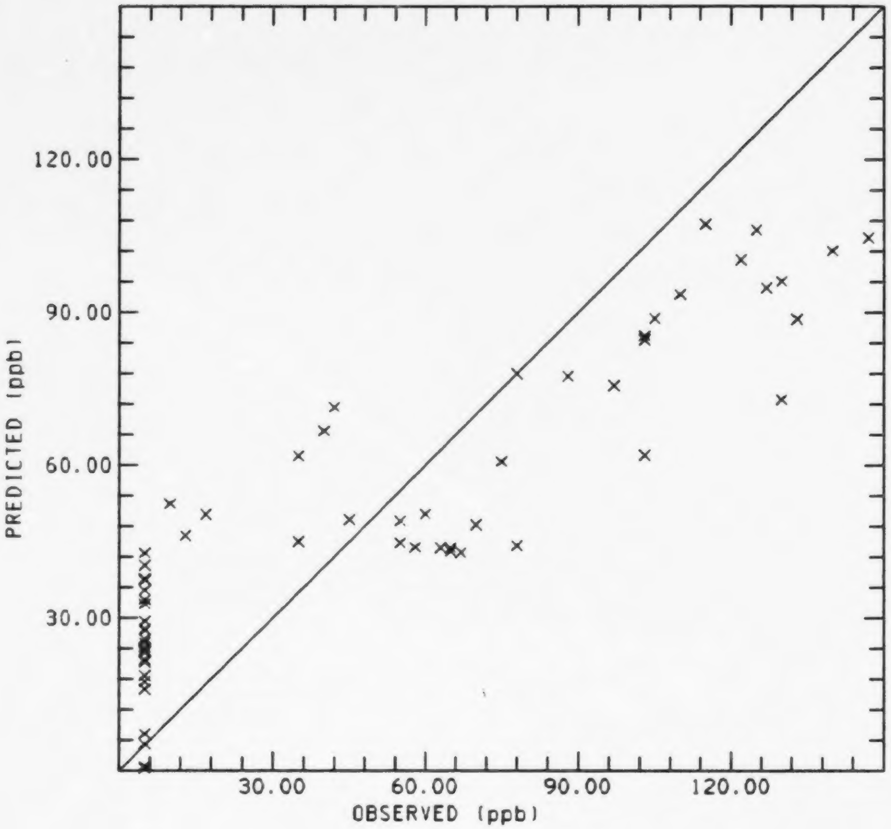
produced improvements in model performance; the point, one-cell search, and two-cell search matches the peak observed observation to within 18, 8, and 5 percent for the DKLB monitor, and 36, 32, and 23 prcent for the DLLS monitors. For the CNYR monitor, it appears the elevated cloud of ozone concentrations is too far north. At the DKLB monitor the predicted ozone concentrations in the general vicinity (i.e., within two grid cells) are in very good agreement with the observed maximum values.

Figure 6 shows a scatter plot and model performance statistics between predicted and observed hourly ozone concentrations for evaluation Run 2. Also contained in Figure 6 are analyses of the residuals of the predicted and observed ozone concentrations. As indicated in Figure 6 and the time series plots in Figure 3, diagnostic run 2 tends to overpredict the nighttime ozone concentrations and underpredict the peak daytime values. As a result, the bias between predicted and observed hourly ozone concentrations is very low (less than 1 percent). However, the gross error (average absolute error) is fairly high (43 percent). The predicted hourly ozone concentrations for diagnostic run 2 follow the diurnal and spatial variations of the observations well, as indicated by the high correlation coefficient of 0.9.

Possible Improvements to Diagnostic Run 2

Improvements in model performance from diagnostic run 2 could be obtained by raising the VOC, NO_x, and ozone boundary conditions, which may be justified based on the underprediction of the ozone at the upwind monitor (DLLS) and the low values current being used. The peak observed ozone concentration at the upwind monitor occurs fairly early in the day (12 noon), which indicates it is probably due to entrainment of an elevated ozone concentration aloft rather than local chemistry.

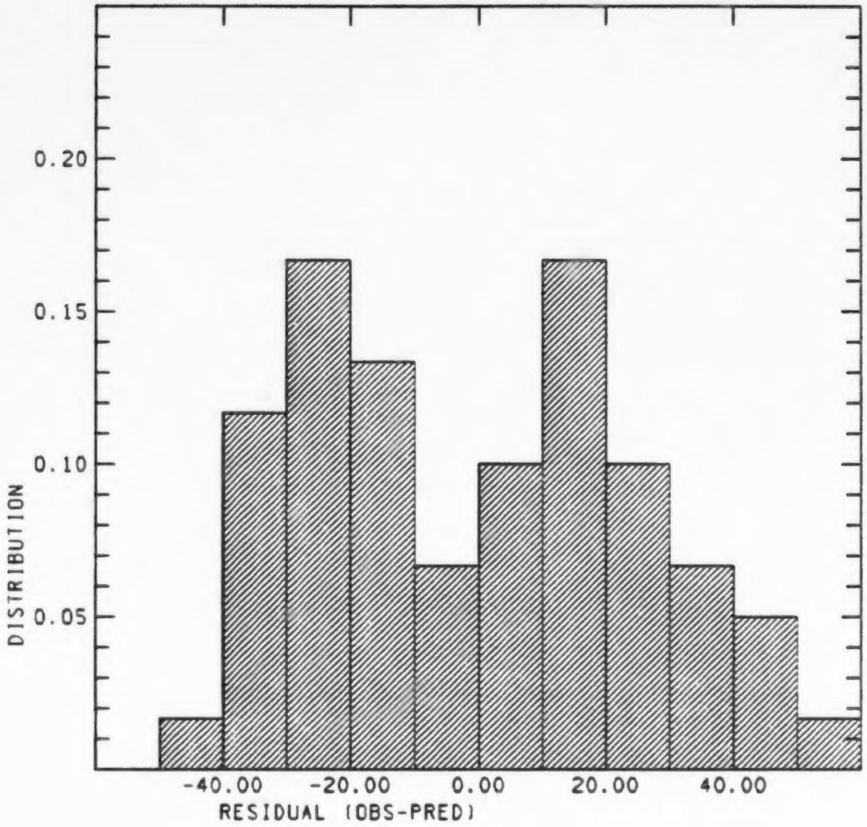
Improvements can also be made in the wind field. The wind field still has a significant southerly component in the late morning and afternoon, which appears to advect the elevated ozone cloud away from the CNYR monitor. Some wind shear is also present between UAM layers 1 and 2, which broadens the ozone peak from the urban emissions, resulting in a lower predicted regional maximum ozone concentration. Since in the afternoon UAM layers 1 and 2 are both contained within the well-mixed layer, one would not expect there to be significant amounts of wind shear between



```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                       OBSERVED        PREDICTED
        AVERAGE        50.39999         50.88372
 STANDARD DEVIATION    47.63355         29.03820
        SKEWNESS       0.51320         0.36600
        KURTOSIS       -1.22432         -0.88317
   OTHER MEASURES
        MEDIAN         40.00000         44.24000
    UPPER QUARTILE     88.00000         72.92999
    LOWER QUARTILE     5.00000         27.54000
     MINIMUM VALUE     5.00000         0.53000
     MAXIMUM VALUE     147.00000          107.30000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED    0.896
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.831 HIGH BOUND 0.937
RATIO OF OVER TO UNDER PREDICTIONS  1.069
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED    38.333
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED    3.333
```

FIGURE 6a. Scatterplot and model performance statistics for hourly ozone concentrations and evaluation run 2 (N = 60).



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THE BINSIZE EQUALS  10.000
```

```
RESIDUAL ANALYSIS

         AVERAGE          -0.48384
  STANDARD DEVIATION      25.16143
         SKEWNESS          0.20968
         KURTOSIS         -1.08769
     OTHER MEASURES
          MEDIAN          -0.21000
      UPPER QUARTILE      18.80000
      LOWER QUARTILE     -22.82000
       MINIMUM VALUE     -42.45000
       MAXIMUM VALUE      57.07001
```

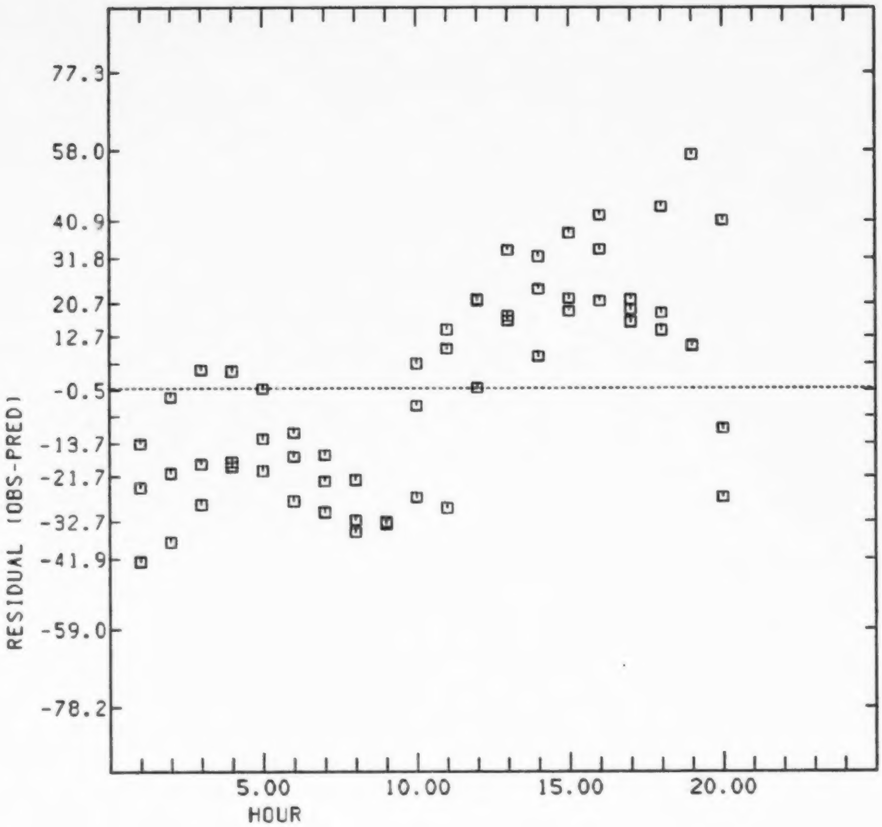
```
BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND -12.5186
UPPER BOUND 11.5509

STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 480.3294
UPPER BOUND 879.6230

THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 24.96
THE AVERAGE ABSOLUTE ERROR IS 21.88

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                              0.9451
RESIDUAL COEFFICIENT OF VARIATION
                              0.4992
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                            - 0.5282
```

FIGURE 6b. Residual analysis of observed minus predicted hourly ozone concentrations for evaluation run 2 (N = 60).



```
THE LINEAR MODEL PARAMETERS
THE CORRELATION IS 0.6804
THE LOWER BOUND IS 0.5155
THE UPPER BOUND IS 0.7967
AT THE 0.0500 PERCENT LEVEL
THE Y-X LINEAR MODEL INTERCEPT IS 10.576
THE Y-X LINEAR MODEL SLOPE IS 0.157
THE X-Y LINEAR MODEL INTERCEPT IS -31.398
THE X-Y LINEAR MODEL SLOPE IS 2.944
```

FIGURE 6c. Plot of residuals versus time of day for evaluation run 2 (N = 60).

these layers. As noted earlier, during 4 June 1984 a high-pressure ridge passed across Atlanta, which resulted in a turning of the winds from the NNE to the SSW. This turning is present in the 0700 and 1900 LST upper-air soundings at Athens, but the exact hours of the turning of the upper-level winds cannot be determined from the hourly surface wind measurements, which are subjected to local influences. The use of linear interpolation of the 0700 and 1900 LST soundings at Athens results in a continuous turning of the wind throughout the day, when in actuality it probably occurs within a few hours as the high-pressure ridge passes through. If the upper-level winds persist with a more northerly component during the morning hours, as is present in the 0700. Athens sounding, and then turns to the SSW in the afternoon, the elevated ozone cloud could then possibly impact the CNYR monitor at the proper time. In addition, use of identical wind fields in layers 1 and 2 during periods of rapid vertical mixing to eliminate the wind shear below the mixing height may result in a sharper predicted peak concentration; the Athens upper-air sounding does support the presence of some wind shear in the mixed-layer.

Another possible explanation for the underprediction of the observed ozone peak at Conyers is that the 1985 NAPAP inventory underestimates the amount of VOC emissions. There are still many uninventoried sources whose individual emissions may be small, but when combined together may produce a significant impact. A further possible reason for the underprediction is that the wind speeds are too high. There has been some discussion that wind speeds reported at FAA sites (instantaneous 1-minute averages) tend to be higher than the hourly integrated values. Thus, as a sensitivity simulation, all observed wind speeds at FAA sites were reduced 50 percent and new UAM wind fields were created. The results of this sensitivity test are discussed in Appendix G.

Although implementation of some of the above changes to the boundary conditions and wind fields would probably improve model performance, the use of those procedures may not be consistent with some of the objectives of this study, namely the demonstration of the PLANR use of the UAM. Thus, since model performance from diagnostic run 2 satisfies the model performance goal, it was deemed a suitable base case. Nevertheless we recommend that when the UAM(CB-IV) and associated preprocessor programs are delivered to the state of Georgia, they should carry out sensitivity studies like those discussed above (and presented in Appendix G), which may improve the UAM inputs data bases and model performance. This exercise will also help them gain experience with the causes and effects of UAM inputs on predicted ozone concentrations.

6 APPLICATION OF THE UAM TO ATLANTA FOR EMISSION REDUCTION SCENARIOS

The UAM was exercised for several different emission scenarios using the UAM modeling inputs corresponding to evaluation run 2. Two base case emission scenarios are used: with biogenic emissions and without biogenic emissions. Different across the board anthropogenic VOC emission reduction scenarios are examined in order to determine what level of anthropogenic VOC emission reductions are required in order to reduce the peak observed ozone concentration of 14.7 pphm to below the NAAQS ozone standard of 12 pphm. The following emission scenarios were used:

- Base case (all anthropogenic emissions) with biogenic emissions
  - 30% reduction in anthropogenic VOC emissions
  - 60% reduction in anthropogenic VOC emissions
  - 90% reduction in anthropogenic VOC emissions

- Base Case (all anthropogenic emissions) without biogenic emissions
  - 30% reduction in anthropogenic emissions
  - 60% reduction in anthropogenic emissions
  - 90% reduction in anthropogenic emissions

TRACER SIMULATION

Before conducting a UAM modeling analysis, it is useful to perform a weighted tracer simulation for the two principle ozone precursors, VOC and NO_x, in order to obtain a rough estimate of contributions of initial concentrations, boundary conditions, and emissions to predicted concentration levels. In a weighted tracer simulation, the UAM is run in an inert mode (i.e., no chemistry or deposition) with several different "colored" tracers (species) that represent the major contributers to VOC and NO_x concentrations within the modeling domain. In the weighted tracer simulation for Atlanta different colored tracers were used for initial concentrations, lateral boundary conditions (four colors, one for each face), top boundary conditions, anthropogenic area source emissions, biogenic area source emissions, and point source emissions.

Appendix F displays the results of this tracer simulation at 0800, 1200, and 1600 LST on 4 June 1984. By 0800 initial concentrations of NO_x (Appendix F-1a) and VOC (Appendix F-2a) are almost completely advected out of the region and only affect the extreme southeastern portion of the modeling domain. By noon (Appendixes F-3 and F-4), initial concentrations have no influence in the modeling domain. At noon, NO_x concentrations are dominated by emissions, where, downwind of Atlanta (i.e., the location of the maximum predicted ozone concentration) area source NO_x contributes over 70 percent, point sources contribute about 20 percent, and boundary NO_x contributes approximately 10 percent. Boundary VOC contributes a higher percentage to the total tracer VOC downwind of Atlanta than seen for NO_x where the percentage contribution of boundary, anthropogenic emissions, and biogenic emissions at 12 noon are approximately 30, 50, and 20 percent. The relative contributions to total NO_x and VOC tracer at 1600 LST is approximately the same as for 12 noon (Appendixes F-5 and F-6).

In regions of the UAM modeling domain away from the influences of emissions from the city of Atlanta, biogenic and boundary VOC dominate the total VOC tracer concentration. Because of the presence of several large power plants within the UAM modeling domain (see Appendixes F-3d and F-5d) the point source NO_x dominates the NO_x tracer concentrations downwind of the power plants and the boundary NO_x concentration does not contribute significantly to NO_x tracer concentrations in the interior of the UAM modeling domain.

UAM MODELING RESULTS

The predicted regional maximum ozone concentration for the base case with and without biogenic emissions are, respectively, 13.22 and 12.28 pphm. The modeling objective is to compare the levels of anthropogenic VOC control (with and without biogenics) required to effect similar percentage reductions in the regional peak ozone changes. Since the base case peaks are dissimilar, the simulations will address the level of reductions required to reduce regional peak ozone by 18.4 percent (equivalent to reducing the observed peak from 14.7 to 12.0 pphm).

Table 6 lists the predicted regional maximum ozone concentrations, percent reduction of the maximum ozone concentration, and the maximum predicted ozone concentration normalized to the observed peak value for each of the emission scenarios. The results from Table 6 are graphically shown in Figure 7. According to Figure 7, to reduce the regional maximum ozone concentration 18.4 percent (i.e., reduce the maximum observation from 14.7 to 12.0 pphm), a 100 and 62 percent control of anthropogenic VOC emissions is required for the cases with and without biogenic emissions, respectively. If one considers the ozone NAAQS as 12.4 pphm, then an 87 and 52 percent control of anthropogenic VOC emissions are required to reduce the predicted regional maximum ozone concentration by 15.6 percent for the, respectively, scenarios with and without biogenic emissions. In either case, the model calculations indicate that the inclusion of biogenic emissions in VOC control strategies for Atlanta on this day results in an additional 35 to 40 percent control on anthropogenic VOC emissions over the case when biogenic emissions are not included.

COMPARISON WITH A PREVIOUS STUDY

As noted previously, a similar analysis of effects of biogenic emissions on VOC control strategies for Atlanta on this day was carried out by Chameides and co-workers using the EKMA model (Chameides et al., 1988). Over the 15-hour EKMA modeling period they estimated biogenic emissions to be 30 kg/km^2 for isoprene, and a total biogenic VOC emission rate of 50 kg/km^2. They also estimated daily total biogenic emission rate of 65 kg/km^2. In their EKMA analysis, biogenic emission rates were varied from zero to 50 kg/km^2 and were assumed to be isoprene. The EPA has summarized biogenic VOC flux rates for 12 other biogenic VOC inventories (EPA, 1984). These values for the other biogenic inventories generally range from 780 to 2,540 μg/m^2-h, with one extreme value at 8,890 μg/m^2-h. The biogenic emission rates

TABLE 6. Regional maximum ozone concentrations (pphm) predicted by the UAM for the different emission scenarios.

	Maximum Ozone Concentration pphm	Percent Reductions from Base Case	Maximum Ozone Normalized to Peak Observation (pphm)
Peak Cbserved	14.7	0.0	14.7
Ozone NAAQS*	12.0	18.4	12.0
With Biogenics			
0% VOC Reduction	13.22	0.0	14.7
30% VOC Reduction	12.68	4.1	14.1
60% VOC Reduction	11.91	9.9	13.2
90% VOC Reduction	11.08	16.2	12.3
Without Biogenics			
0% VOC Reduction	12.28	0.0	14.7
30% VOC Reduction	11.16	9.1	13.4
60% VOC Reduction	10.09	17.8	12.1
90% VOC Reduction	8.98	26.9	10.7

* Technically, the ozone NAAQS is 0.12 ppm rounded. Thus, an ozone concentration of 12.4 pphm (15.6% reduction from observed peak) is considered attainment.

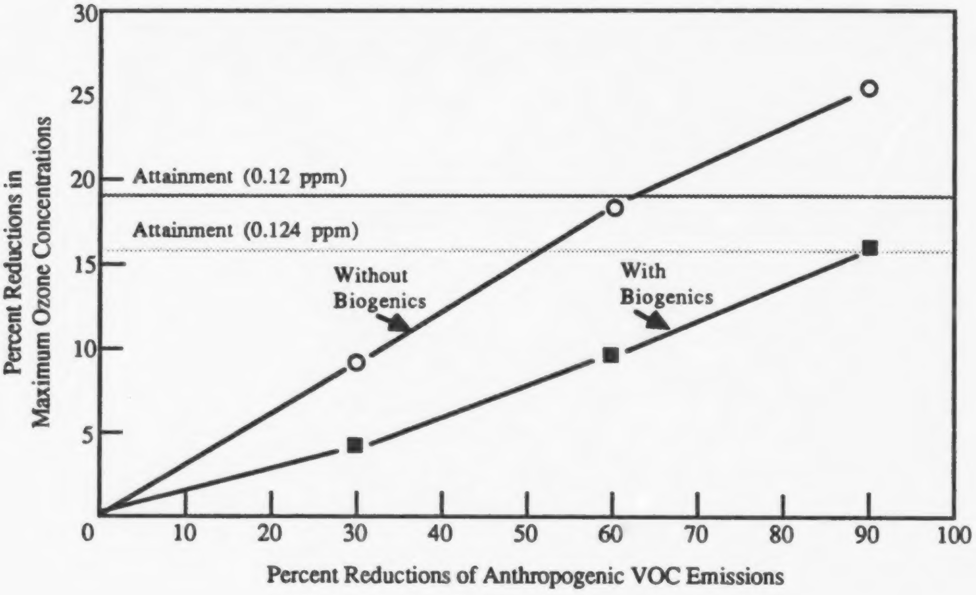


FIGURE 7. Relationship between percent reduction of anthropogenic VOC emissions to percent reduction of the regional maximum ozone concentration with and without biogenic emissions.

of 30, 50, and 65 kg/km^2 reported by Chameides and co-workers translate into biogenic flux rates of 2,000, 3,333, and 2,708 $\mu g/m^2$-h. (Note that the 65 kg/km^2 is a daily total.) In our study we used a 24-hour average biogenic emission flux for the UAM modeling domain of 2,197 $\mu g/m^2$-h. Thus our study and the work of Chameides and co-workers used similar estimates of biogenic emission flux rates that are on the high end, but well within the range of biogenic fluxes of other studies (EPA, 1984). Due to the large amount of foliage in the Southeast, it is expected that biogenic emission fluxes for the Atlanta region are on the high end of continental flux estimates.

However, there are some differences in the emissions used in this study and those used in the work of Chameidies and co-workers. These differences include the speciation of the biogenic emissions into CB-IV species and the total anthropogenic VOC and NO_x emissions used. Chameides and co-workers assumed that all of the biogenic emissions were isoprene in their EKMA analysis, whereas our study assumed that isoprene made up only 19 percent by weight of the 24-hour total biogenic emissions. (Note that isoprene contributed about 25 percent of the total biogenics for the 15 daylight hours.) The less reactive CB-IV species PAR made up the largest portion of the biogenic emissions in this study (65 percent by weight), with the remainder of the biogenic emissions assumed to be the CB-IV species OLE. Since isoprene is much more reactive than PAR, Chameides and co-workers used a more reactive biogenic emissions inventory than was used in our study.

Chameides and co-workers estimated that without biogenic emissions, a 30 percent reduction of anthropogenic emissions is required in order to reduce the maximum observed ozone concentration of 14.7 to 12.0 pphm. In contrast, we estimated that a 62 percent control of anthropogenic VOC emissions is required to reduce the maximum observed value from 14.7 to 12.0 pphm without biogenics. There may be several reasons for the differences in VOC emission control requirements predicted by the UAM and EKMA.

(1) A lower base case maximum daily ozone concentration (12.28 pphm) was used in UAM than was used in the EKMA (14.7 pphm). Thus, a larger percentage of the UAM-predicted maximum daily ozone concentration is due to background concentrations, which will not be affected by emission control strategies.

(2) The UAM was exercised with boundary conditions that reflected the presence of upwind emission sources (anthropogenic and biogenic). Thus, again, a larger fraction of the UAM-predicted maximum daily ozone concentration is due to background, which will not be affected by anthropogenic VOC reductions.

(3) Due to changes in the reactivity and chemistry of the atmosphere in the different emission reduction scenarios, the regional maximum ozone concentration predicted by the UAM does not occur at the same location in each scenario. If changes in emissions causes the maximum ozone concentration to lie outside of the EKMA trajectory, then the maximum observed ozone cannot be simulated by EKMA, and EKMA will overstate the ozone reductions due to the emission reductions.

(4) The observed vertical wind profile at Athens, Georgia and the UAM layer 1 and 2 wind fields both exhibit some wind shear in the mixed-layer. This wind shear, which cannot be simulated by EKMA, results in a larger portion of the predicted maximum ozone concentration being attributable to background conditions rather than to urban emissions from Atlanta.

(5) The UAM modeling analysis included the emissions from several large power plants in the region (50 percent of the NO_x inventory) that were not accounted for in the EKMA analysis. These NO_x emissions combined with the background VOC concentrations may produce ozone concentrations that will not be affected by the anthropogenic VOC emission reductions.

(6) The anthropogenic emission inventory used in this study most probably underestimates actual anthropogenic VOC emissions. The annual NAPAP inventory, which is probably an underestimate to begin with, is adjusted to a typical summer weekday based on average summer conditions. Ozone episodes tend to be highly correlated with hotter than normal temperatures, although 4 June 1984 was not an excessively hot day. Except for mobile sources, which were adjusted to episodic temperature conditions based on

MOBILE-4, VOC emissions (e.g., solvent use and other evaporative emissions) were not adjusted to the higher emission rates expected on a hotter than normal day.

(7) The wind speeds may be too high in the UAM simulation, causing excessive dilution of the urban plume.

Of particular note in these differences is the underprediction of the observed peak ozone concentration (14.7 pphm) by the UAM in evaluation run 2 (13.2 pphm). To investigate this effect, a sensitivity test reduced the observed wind speeds at some of the surface sites. The results of this sensitivity test are discussed in Appendix G.

Despite the differences between our study and the study reported by Chameides and co-workers (1988), both studies conclude that by including biogenic emissions in an attainment demonstration for Atlanta for June 4 1984, an additional 35 to 40 percent anthropogenic emission reduction over the case without biogenics is required to meet attainment of the ozone NAAQS. Chameides and co-workers report that the anthropogenic VOC emission control requirements increase from 30 to 70 percent, whereas we report that an increase from 62 to 100 percent is needed. However, because the UAM underpredicts the peak observed ozone concentration, and for the reasons cited above, it is probable that the UAM is overstating the VOC emission control requirements.

DISCUSSION

There were two main objectives of this study: (1) the demonstration of the PLANR use of the UAM for the city of Atlanta, and (2) the analysis of the effects of biogenic emissions on VOC control strategies. Using only routinely available data, it has be shown that adequate UAM modeling inputs can be created using objective techniques and a minimal amount of diagnostic simulations. It has also been demonstrated that biogenic emissions do affect VOC control strategies for ozone attainment. However, in a sense these two objectives are not entirely consistent with each other, since more accurate results of the effects of biogenic emissions on ozone attainment demonstration would most likely be obtained if the UAM base case simulation exhibited better model performance. Improved UAM modeling inputs could be generated either by using data from an intensive measurement network or through modifying the existing inputs by an experienced UAM model user. However, neither of these approaches is consistent with the demonstration of the PLANR use of the UAM. Because of this conflict of objectives, additional uncertainties are introduced into the analysis of the effects of biogenic. These uncertainties are addressed somewhat in the sensitivity analysis discussed in Appendix G.

As noted previously, several other sources of uncertainity in the analysis need to be recognized when interpreting the results. Foremost among these are the uncertainties in the biogenic and anthropogenic emission inventories. These uncertainties may be biased in such a fashion that the calculated effects of biogenic emissions presented here possibly are overestimates of the actual effects. This is because the biogenic VOC emissions may be overestimates of actual emissions, and the anthropogenic VOC emissions are most likely underestimates of actual emissions. Recent analysis of biogenic emissions have indicated that 15 to 35 percent of the biogenic emissions are reacted away before leaving the forest canopy, thus those emissions cannot contribute to the formation of ozone. The 1985 NAPAP inventory only included major VOC emission sources; smaller sources, such as small evaporative sources whose annual emission rate was lower than the cutoff, were not included in the analysis. Many of these smaller sources have peak emission rate during the summer. The uncertainties in the emission inventories contribute substantially to the uncertainties in this analysis. It is expected that use of a better quality anthropogenic emission inventory, representative of actual emission rates, will not only lessen the uncertainties in the analysis of the effects of biogenic emissions, but will also improve model performance of the base case.

Even with the uncertainties in the modeling analysis presented here, two important conclusions can be drawn concerning attainment of the ozone standard for the city of Atlanta. First, biogenic emissions do contribute to some extent to VOC concentrations in the Atlanta region and therefore may lessen the effects of ozone attainment strategies aimed solely at reducing VOC emissions. Although it is suspected that the results presented here are overestimates (i.e., the actual effects of biogenic emissions may be less than presented here), biogenic emissions should be recognized in future modeling studies. The second major conclusion is that a high-quality emission inventory that represents actual emission rates is needed to properly calculate the effects of emission reduction strategies.

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Appendix A

EMISSIONS DATA USED IN THE APPLICATION OF THE UAM TO ATLANTA

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                         Emissions type: Total Merged by Source Category (tons/day) for day 84155
CODE  Source Name                                     THC        RHC        CO         NOx        SOx        TSP
====  =============                                =========  =========  =========  =========  =========  =========

100   FUEL COMBUSTION                                   0.00       0.00       0.00       0.00       0.00       0.00
110        AGRICULTURAL                                 0.00       0.00       0.00       0.00       0.00       0.00
120        OIL AND GAS PRODUCTION                       0.00       0.00       0.00       0.00       0.00       0.00
130        PETROLEUM REFINING                           0.00       0.00       0.01       0.08       0.08       0.01
140        OTHER MANUFACTURING/INDUSTRIAL               0.55       0.22       1.37       8.10       4.12       0.58
150        ELECTRIC UTILITIES                           0.02       0.01       0.06       1.38       0.16       0.04
160        OTHER SERVICES AND COMMERCE                  0.14       0.06       0.58       2.85       1.83       0.18
170        RESIDENTIAL                                  0.18       0.01       0.70       3.44       0.17       0.11
199        OTHER                                        0.00       0.00       0.00       0.00       0.00       0.00
200   WASTE BURNING                                     0.00       0.00       0.00       0.00       0.00       0.00
210        AGRICULTURAL DEBRIS                          0.70       0.55       4.11       0.09       0.00       0.62
220        RANGE MANAGEMENT                             0.00       0.00       0.00       0.00       0.00       0.00
230        FOREST MANAGEMENT                            0.00       0.00       0.00       0.00       0.00       0.00
240        INCINERATION                                 2.73       0.36       7.93       0.05       0.03       0.98
299        OTHER                                       16.58      16.26      46.93       2.78       0.40      10.67
300   SOLVENT USE                                       0.00       0.00       0.00       0.00       0.00       0.00
310        DRY CLEANING                                 4.80       2.44       0.00       0.00       0.00       0.00
320        DEGREASING                                   7.14       6.03       0.00       0.00       0.00       0.00
330        ARCHITECTURAL COATING                       19.57      18.60       0.00       0.00       0.00       0.00
340        OTHER SURFACE COATING                       65.04      63.87       0.00       0.00       0.00       0.87
350        ASPHALT PAVING                               0.00       0.00       0.00       0.00       0.00       0.00
360        PRINTING                                    13.92      11.21       0.00       0.00       0.00       0.00
370        DOMESTIC                                     0.00       0.00       0.00       0.00       0.00       0.00
380        INDUSTRIAL SOLVENT USE                       0.00       0.00       0.00       0.00       0.00       0.00
399        OTHER                                       75.41      55.22       0.00       0.00       0.00       0.00
400   PETROLEUM PROCESS, STORAGE & TRANSFER             0.00       0.00       0.00       0.00       0.00       0.00
410        OIL AND GAS EXTRACTION                      12.61       4.89       0.00       0.00       0.00       0.00
420        PETROLEUM REFINING                          13.35       9.86       0.15       0.00       0.00       0.05
430        PETROLEUM MARKETING                         33.98      32.85       0.00       0.00       0.00       0.00
499        OTHER                                        0.00       0.00       0.00       0.00       0.00       0.00
500   INDUSTRIAL PROCESSES                              0.00       0.00       0.00       0.00       0.00       0.00
510        CHEMICAL                                    15.12      10.01       0.00       0.10       6.07       0.25
520        FOOD AND AGRICULTURAL                        0.87       0.58       0.00       0.00       0.00       0.00
560        MINERAL PROCESSES                            1.96       1.46       0.17       6.00       4.55       3.55
570        METAL PROCESSES                              2.98       2.93       0.04       0.02       4.11       1.29
580        WOOD AND PAPER                              18.83      18.52       0.00       0.02       0.01       0.97
599        OTHER                                       62.67      50.01       0.00       0.00       0.00       0.00
600   MISC PROCESSES                                    0.00       0.00       0.00       0.00       0.00       0.00
610        PESTICIDE APPLICATION                        0.00       0.00       0.00       0.00       0.00       0.00
620        FARMING OPERATIONS                           0.00       0.00       0.00       0.00       0.00       0.00
630        CONSTRUCTION AND DEMOLITION                  0.00       0.00       0.00       0.00       0.00       0.00
640        ENTRAINED ROAD DUST - PAVED                  0.00       0.00       0.00       0.00       0.00       0.00
650        ENTRAINED ROAD DUST - UNPAVED                0.00       0.00       0.00       0.00       0.00       0.00
660        UNPLANNED FIRES                              1.69       1.33       7.70       0.18       0.00       1.77
680        WASTE DISPOSAL                               0.78       0.31       0.00       0.00       0.00       0.00
685        NATURAL SOURCES                              0.00       0.00       0.00       0.00       0.00       0.00
699        OTHER                                        0.32       0.24       0.02       0.02       0.01       0.47
700   ON ROAD VEHICLES                                  0.00       0.00       0.00       0.00       0.00       0.00
710        LIGHT DUTY PASSENGER                       580.06     547.14    1454.22     156.13       9.42     133.86
720        LIGHT AND MEDIUM DUTY TRUCKS               113.24     106.19     311.91      38.63       2.87      29.76
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                                       Emissions type: Total Merged by Source Category (tons/day) for day 84155
CODE  Source Name                                              THC        RHC        CO         NOx        SOx        TSP
====  =============                                         =========  =========  =========  =========  =========  =========

730        HEAVY DUTY GAS TRUCKS                               32.33      30.53     163.35      12.75       0.63       4.87
740        HEAVY DUTY DIESEL TRUCKS                            13.71      12.41      50.36     121.06      14.48      29.01
750        MOTORCYCLES                                          0.00       0.00       0.00       0.00       0.00       0.00
799        OTHER                                                0.00       0.00       0.00       0.00       0.00       0.00
800   OTHER MOBILE                                              0.00       0.00       0.00       0.00       0.00       0.00
810        OFF ROAD VEHICLES                                    0.00       0.00       0.00       0.00       0.00       0.00
820        TRAINS                                               4.29       3.89       6.71      19.11       2.94       1.29
830        SHIPS                                                5.82       5.49      17.95       0.23       0.04       0.00
850        AIRCRAFT - GOVERNMENT                                1.17       0.97       2.19       0.47       0.06       0.93
860        AIRCRAFT - OTHER                                     7.90       6.51      42.84       9.39       1.01       0.48
870        MOBILE EQUIPMENT                                     0.00       0.00       0.00       0.00       0.00       0.00
880        UTILITY EQUIPMENT                                    0.00       0.00       0.00       0.00       0.00       0.00
891     SEEPS/BIOGENIC                                          0.00       0.00       0.00       0.00       0.00       0.00
892     CHANNEL SHIPPING                                        0.00       0.00       0.00       0.00       0.00       0.00
893     OCS AND RELATED SOURCES                                 0.00       0.00       0.00       0.00       0.00       0.00
894     TIDELAND PLATFORMS                                      0.00       0.00       0.00       0.00       0.00       0.00
900     UNSPECIFIED SOURCES                                    11.40       9.52      27.82     367.91    2065.01      50.77

TOTAL ANTHROPOGENIC EMISSIONS                                1141.89    1030.45    2147.11     750.79    2118.01     273.41

TOTAL BIOGENIC EMISSIONS                                     1487.84    1487.84       0.00       0.00       0.00       0.00

TOTAL ANTHROPOGENIC + BIOGENIC                               2629.73    2518.29    2147.11     750.79    2118.01     273.41
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                                   Emissions type: Total Merged by Source Category (tons/day) for day 84155
CODE  Source Name                                     OLE        PAR        TOL        XYL       FORM
====  =============                               =========  =========  =========  =========  =========
100   FUEL COMBUSTION                                 0.00       0.00       0.00       0.00       0.00
110        AGRICULTURAL                               0.00       0.00       0.00       0.00       0.00
120        OIL AND GAS PRODUCTION                     0.00       0.00       0.00       0.00       0.00
130        PETROLEUM REFINING                         0.00       0.00       0.00       0.00       0.00
140        OTHER MANUFACTURING/INDUSTRIAL             0.01       0.08       0.00       0.00       0.01
150        ELECTRIC UTILITIES                         0.00       0.01       0.00       0.00       0.00
160        OTHER SERVICES AND COMMERCE                0.00       0.05       0.00       0.00       0.01
170        RESIDENTIAL                                0.00       0.01       0.00       0.00       0.00
199        OTHER                                      0.00       0.00       0.00       0.00       0.00
200   WASTE BURNING                                   0.00       0.00       0.00       0.00       0.00
210        AGRICULTURAL DEBRIS                        0.03       0.38       0.00       0.00       0.00
220        RANGE MANAGEMENT                           0.00       0.00       0.00       0.00       0.00
230        FOREST MANAGEMENT                          0.00       0.00       0.00       0.00       0.00
240        INCINERATION                               0.01       0.08       0.00       0.00       0.00
299        OTHER                                      2.07      10.94       0.00       0.00       0.00
300   SOLVENT USE                                     0.00       0.00       0.00       0.00       0.00
310        DRY CLEANING                               0.03       2.09       0.14       0.17       0.00
320        DEGREASING                                 0.04       3.45       1.29       0.59       0.00
330        ARCHITECTURAL COATING                      0.76      13.52       3.58       0.60       0.00
340        OTHER SURFACE COATING                      0.34      29.94      24.49       8.05       0.00
350        ASPHALT PAVING                             0.00       0.00       0.00       0.00       0.00
360        PRINTING                                   0.02      11.05       0.12       0.00       0.00
370        DOMESTIC                                   0.00       0.00       0.00       0.00       0.00
380        INDUSTRIAL SOLVENT USE                     0.00       0.00       0.00       0.00       0.00
399        OTHER                                      0.00      29.75       0.00       0.00       0.31
400   PETROLEUM PROCESS, STORAGE & TRANSFER           0.00       0.00       0.00       0.00       0.00
410        OIL AND GAS EXTRACTION                     0.00       4.89       0.00       0.00       0.00
420        PETROLEUM REFINING                         0.18       8.74       0.06       0.31       0.57
430        PETROLEUM MARKETING                        0.72      16.05       6.59       9.00       0.02
499        OTHER                                      0.00       0.00       0.00       0.00       0.00
500   INDUSTRIAL PROCESSES                            0.00       0.00       0.00       0.00       0.00
510        CHEMICAL                                   1.25       4.93       1.24       0.11       0.09
520        FOOD AND AGRICULTURAL                      0.06       0.35       0.05       0.01       0.01
560        MINERAL PROCESSES                          0.05       1.22       0.02       0.12       0.02
570        METAL PROCESSES                            0.00       1.34       1.27       0.28       0.00
580        WOOD AND PAPER                             0.01       8.44       8.01       1.75       0.00
599        OTHER                                      8.10      30.72       6.00       0.51       0.51
600   MISC PROCESSES                                  0.00       0.00       0.00       0.00       0.00
610        PESTICIDE APPLICATION                      0.00       0.00       0.00       0.00       0.00
620        FARMING OPERATIONS                         0.00       0.00       0.00       0.00       0.00
630        CONSTRUCTION AND DEMOLITION                0.00       0.00       0.00       0.00       0.00
640        ENTRAINED ROAD DUST - PAVED                0.00       0.00       0.00       0.00       0.00
650        ENTRAINED ROAD DUST - UNPAVED              0.00       0.00       0.00       0.00       0.00
660        UNPLANNED FIRES                            0.07       0.92       0.00       0.00       0.00
680        WASTE DISPOSAL                             0.04       0.20       0.00       0.00       0.00
685        NATURAL SOURCES                            0.00       0.00       0.00       0.00       0.00
699        OTHER                                      0.02       0.15       0.02       0.01       0.00
700   ON ROAD VEHICLES                                0.00       0.00       0.00       0.00       0.00
710        LIGHT DUTY PASSENGER                      16.14     385.49      58.29      52.64       1.43
720        LIGHT AND MEDIUM DUTY TRUCKS               3.29      73.96      11.12      10.54       0.31
```
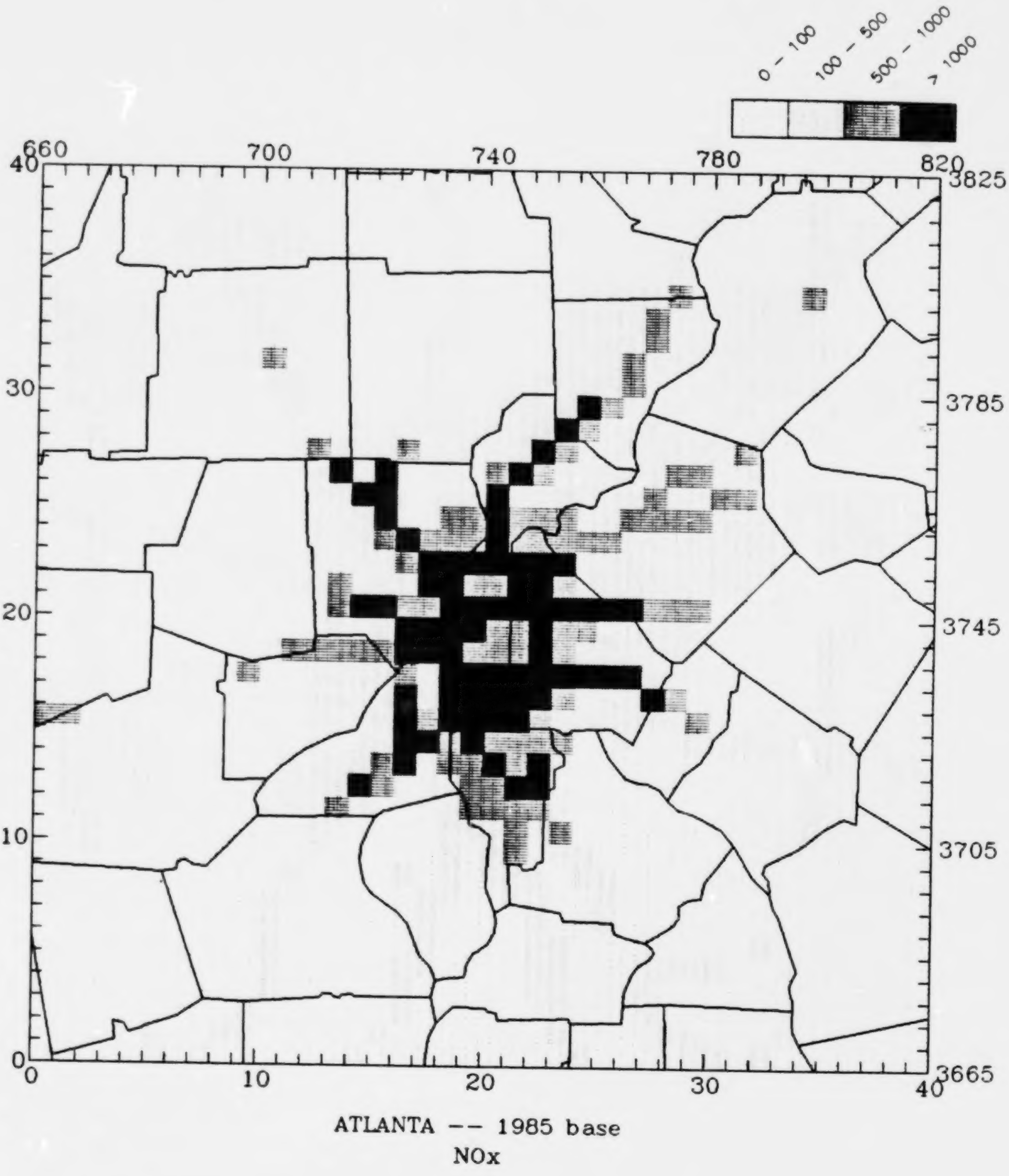

```
                                                     Emissions type: Total Merged by Source Category (tons/day) for day 84155
CODE   Source Name                                                      OLE        PAR        TOL        XYL        FORM
====   =============                                                 =========  =========  =========  =========  =========
730         HEAVY DUTY GAS TRUCKS                                       0.77      23.21       1.47       2.12       0.07
740         HEAVY DUTY DIESEL TRUCKS                                    0.76       6.66       2.95       0.27       0.71
750         MOTORCYCLES                                                 0.00       0.00       0.00       0.00       0.00
799         OTHER                                                       0.00       0.00       0.00       0.00       0.00
800    OTHER MOBILE                                                     0.00       0.00       0.00       0.00       0.00
810         OFF ROAD VEHICLES                                           0.00       0.00       0.00       0.00       0.00
820         TRAINS                                                      0.24       2.09       0.92       0.08       0.22
830         SHIPS                                                       0.14       4.15       0.27       0.39       0.01
850         AIRCRAFT - GOVERNMENT                                       0.13       0.31       0.02       0.02       0.13
860         AIRCRAFT - OTHER                                            0.88       2.22       0.14       0.14       0.86
870         MOBILE EQUIPMENT                                            0.00       0.00       0.00       0.00       0.00
880         UTILITY EQUIPMENT                                           0.00       0.00       0.00       0.00       0.00
891     SEEPS/BIOGENIC                                                  0.00       0.00       0.00       0.00       0.00
892     CHANNEL SHIPPING                                                0.00       0.00       0.00       0.00       0.00
893     OCS AND RELATED SOURCES                                         0.00       0.00       0.00       0.00       0.00
894     TIDELAND PLATFORMS                                              0.00       0.00       0.00       0.00       0.00
900     UNSPECIFIED SOURCES                                             0.52       5.97       0.70       1.12       0.14

TOTAL ANTHROPOGENIC EMISSIONS                                          36.65     683.35     128.77      88.83       5.45

TOTAL BIOGENIC EMISSIONS                                              242.34     969.40       0.00       0.00       0.00

TOTAL ANTHROPOGENIC + BIOGENIC                                        278.99    1652.75     128.77      88.83       5.45
```

```
                                          Emissions type: Total Merged by Source Category (tons/day) for day 84155

CODE  Source Name                                   ALD2      ETH       MEOH      ETOH      ISOP
====  =============                              ========= ========= ========= ========= =========
100   FUEL COMBUSTION                                0.00      0.00      0.00      0.00      0.00
110        AGRICULTURAL                              0.00      0.00      0.00      0.00      0.00
120        OIL AND GAS PRODUCTION                    0.00      0.00      0.00      0.00      0.00
130        PETROLEUM REFINING                        0.00      0.00      0.00      0.00      0.00
140        OTHER MANUFACTURING/INDUSTRIAL            0.00      0.08      0.00      0.05      0.00
150        ELECTRIC UTILITIES                        0.00      0.00      0.00      0.00      0.00
160        OTHER SERVICES AND COMMERCE               0.00      0.00      0.00      0.00      0.00
170        RESIDENTIAL                               0.00      0.00      0.00      0.00      0.00
199        OTHER                                     0.00      0.00      0.00      0.00      0.00
200   WASTE BURNING                                  0.00      0.00      0.00      0.00      0.00
210        AGRICULTURAL DEBRIS                       0.00      0.14      0.00      0.00      0.00
220        RANGE MANAGEMENT                          0.00      0.00      0.00      0.00      0.00
230        FOREST MANAGEMENT                         0.00      0.00      0.00      0.00      0.00
240        INCINERATION                              0.00      0.26      0.00      0.00      0.00
299        OTHER                                     0.00      3.25      0.00      0.00      0.00
300   SOLVENT USE                                    0.00      0.00      0.00      0.00      0.00
310        DRY CLEANING                              0.00      0.00      0.00      0.00      0.00
320        DEGREASING                                0.04      0.61      0.00      0.00      0.00
330        ARCHITECTURAL COATING                     0.14      0.00      0.00      0.00      0.00
340        OTHER SURFACE COATING                     1.05      0.00      0.00      0.00      0.00
350        ASPHALT PAVING                            0.00      0.00      0.00      0.00      0.00
360        PRINTING                                  0.03      0.00      0.00      0.00      0.00
370        DOMESTIC                                  0.00      0.00      0.00      0.00      0.00
380        INDUSTRIAL SOLVENT USE                    0.00      0.00      0.00      0.00      0.00
399        OTHER                                     0.00      0.00      0.00     25.15      0.00
400   PETROLEUM PROCESS, STORAGE & TRANSFER          0.00      0.00      0.00      0.00      0.00
410        OIL AND GAS EXTRACTION                    0.00      0.00      0.00      0.00      0.00
420        PETROLEUM REFINING                        0.00      0.00      0.00      0.00      0.00
430        PETROLEUM MARKETING                       0.46      0.00      0.00      0.00      0.00
499        OTHER                                     0.00      0.00      0.00      0.00      0.00
500   INDUSTRIAL PROCESSES                           0.00      0.00      0.00      0.00      0.00
510        CHEMICAL                                  0.31      1.80      0.26      0.02      0.00
520        FOOD AND AGRICULTURAL                     0.01      0.07      0.01      0.01      0.00
560        MINERAL PROCESSES                         0.00      0.02      0.00      0.00      0.00
570        METAL PROCESSES                           0.05      0.00      0.00      0.00      0.00
580        WOOD AND PAPER                            0.30      0.00      0.00      0.00      0.00
599        OTHER                                     0.62      2.86      0.38      0.30      0.00
600   MISC PROCESSES                                 0.00      0.00      0.00      0.00      0.00
610        PESTICIDE APPLICATION                     0.00      0.00      0.00      0.00      0.00
620        FARMING OPERATIONS                        0.00      0.00      0.00      0.00      0.00
630        CONSTRUCTION AND DEMOLITION               0.00      0.00      0.00      0.00      0.00
640        ENTRAINED ROAD DUST - PAVED               0.00      0.00      0.00      0.00      0.00
650        ENTRAINED ROAD DUST - UNPAVED             0.00      0.00      0.00      0.00      0.00
660        UNPLANNED FIRES                           0.00      0.33      0.00      0.00      0.00
680        WASTE DISPOSAL                            0.00      0.08      0.00      0.00      0.00
685        NATURAL SOURCES                           0.00      0.00      0.00      0.00      0.00
699        OTHER                                     0.01      0.01      0.00      0.00      0.00
700   ON ROAD VEHICLES                               0.00      0.00      0.00      0.00      0.00
710        LIGHT DUTY PASSENGER                     15.58     17.21      0.00      0.00      0.36
720        LIGHT AND MEDIUM DUTY TRUCKS              3.10      3.80      0.00      0.00      0.08
```

```
                                       Emissions type: Total Merged by Source Category (tons/day) for day 84155
CODE   Source Name                                       ALD2      ETH       MEOH      ETOH      ISOP
====   =============                                  ========= ========= ========= ========= =========
730         HEAVY DUTY GAS TRUCKS                        1.49      1.37      0.00      0.00      0.03
740         HEAVY DUTY DIESEL TRUCKS                     0.66      0.40      0.00      0.00      0.00
750         MOTORCYCLES                                  0.00      0.00      0.00      0.00      0.00
799         OTHER                                        0.00      0.00      0.00      0.00      0.00
800    OTHER MOBILE                                      0.00      0.00      0.00      0.00      0.00
810         OFF ROAD VEHICLES                            0.00      0.00      0.00      0.00      0.00
820         TRAINS                                       0.21      0.12      0.00      0.00      0.00
830         SHIPS                                        0.26      0.26      0.00      0.00      0.01
850         AIRCRAFT - GOVERNMENT                        0.08      0.27      0.00      0.00      0.00
860         AIRCRAFT - OTHER                             0.54      1.74      0.00      0.00      0.00
870         MOBILE EQUIPMENT                             0.00      0.00      0.00      0.00      0.00
880         UTILITY EQUIPMENT                            0.00      0.00      0.00      0.00      0.00
891     SEEPS/BIOGENIC                                   0.00      0.00      0.00      0.00      0.00
892     CHANNEL SHIPPING                                 0.00      0.00      0.00      0.00      0.00
893     OCS AND RELATED SOURCES                          0.00      0.00      0.00      0.00      0.00
894     TIDELAND PLATFORMS                               0.00      0.00      0.00      0.00      0.00
900     UNSPECIFIED SOURCES                              1.02      0.03      0.04      0.00      0.00

TOTAL ANTHROPOGENIC                                     25.99     34.71      0.68     25.54      0.48

TOTAL BIOGENIC                                           0.00      0.00      0.00      0.00    276.09

TOTAL ANTHROPOGENIC + BIOGENIC                          25.99     34.71      0.68     25.54    276.57
```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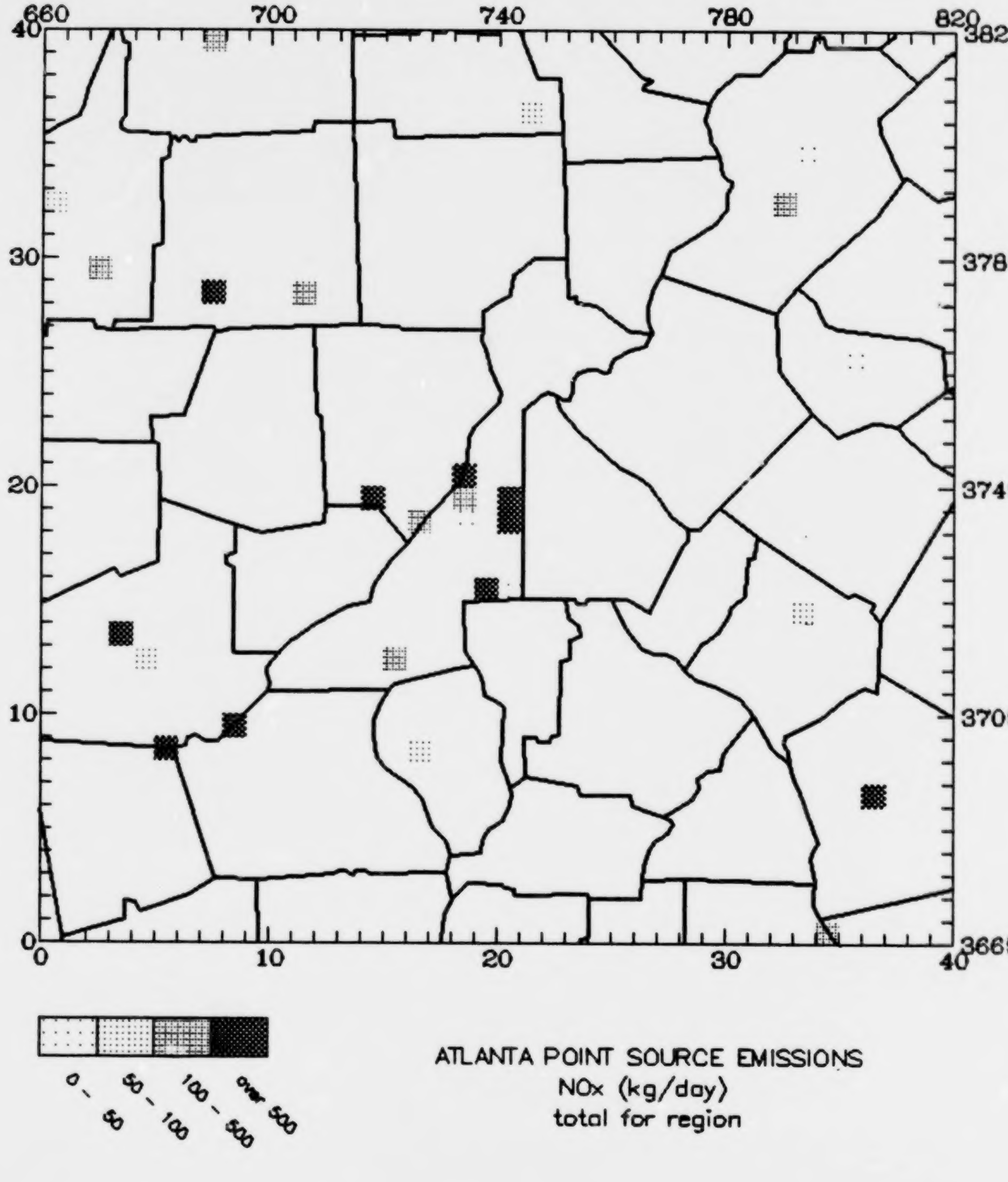
500 - 1000
> 1000
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
ATLANTA -- 1985 base
NOx

Area source and low-level point source NO_x emissions (kg/day)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780
820
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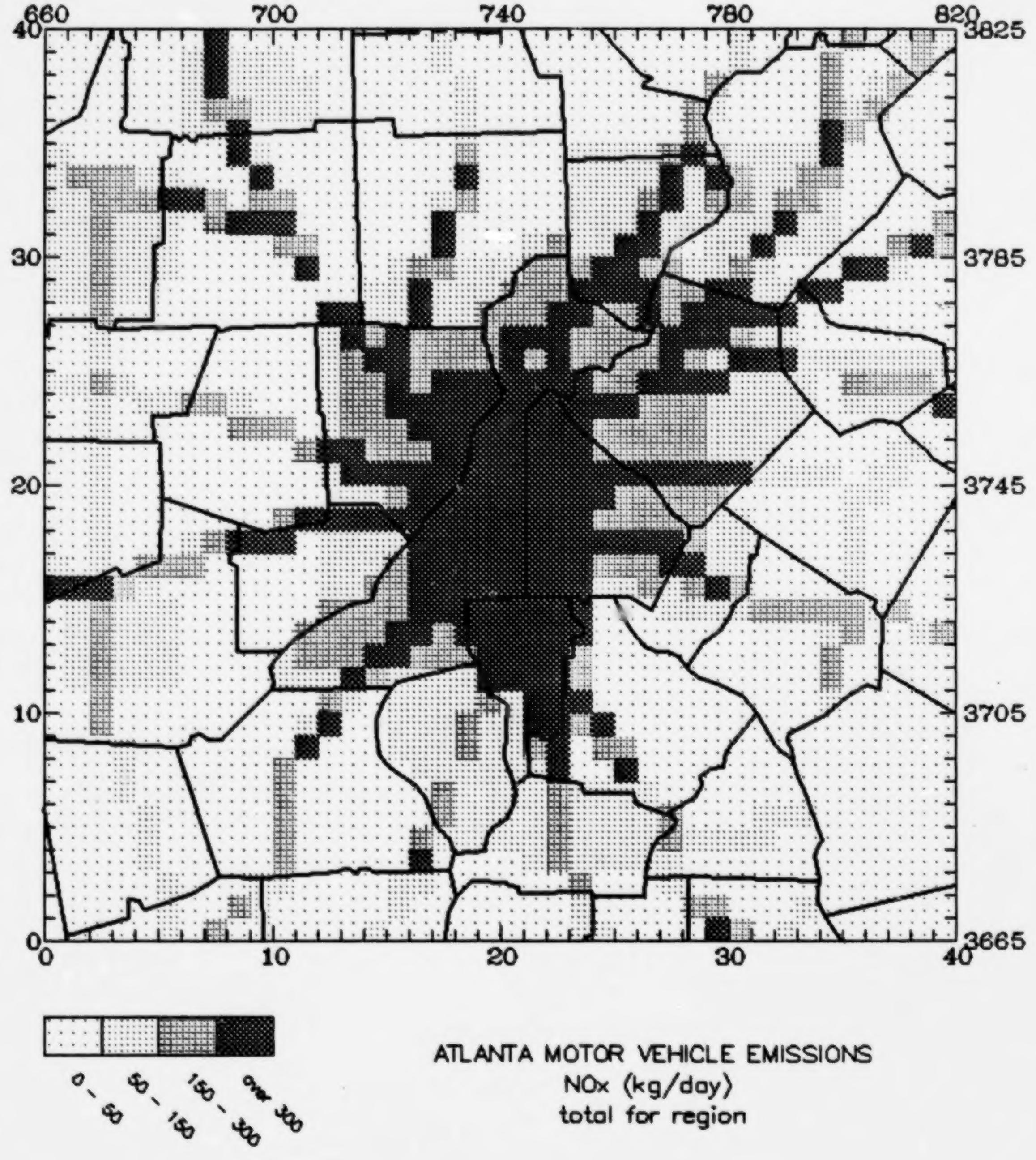
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
0 - 50
50 - 100
100 - 500
over 500

ATLANTA POINT SOURCE EMISSIONS
NOx (kg/day)
total for region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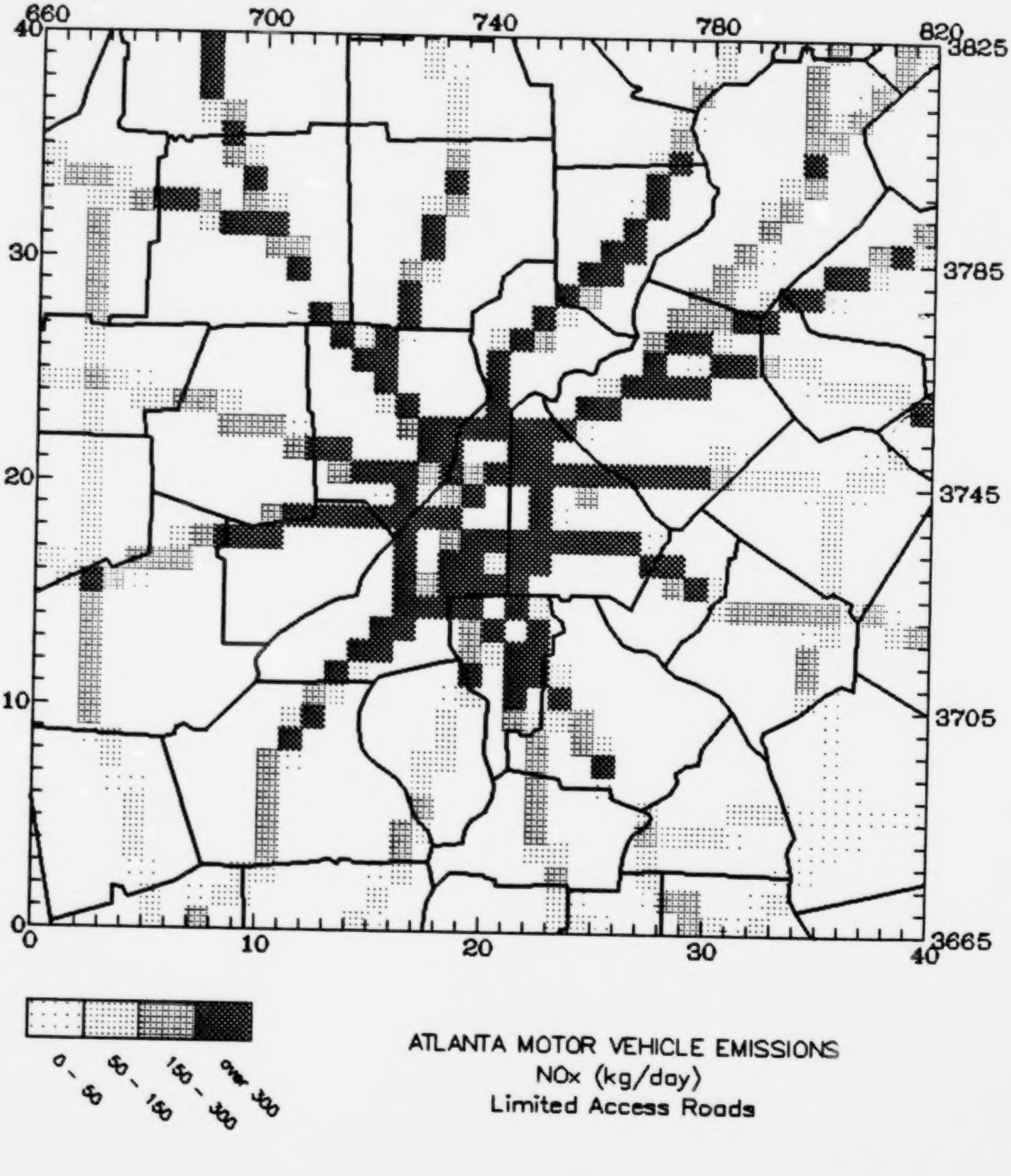
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
0 - 50
50 - 150
150 - 300
over 300

ATLANTA MOTOR VEHICLE EMISSIONS
NOx (kg/day)
total for region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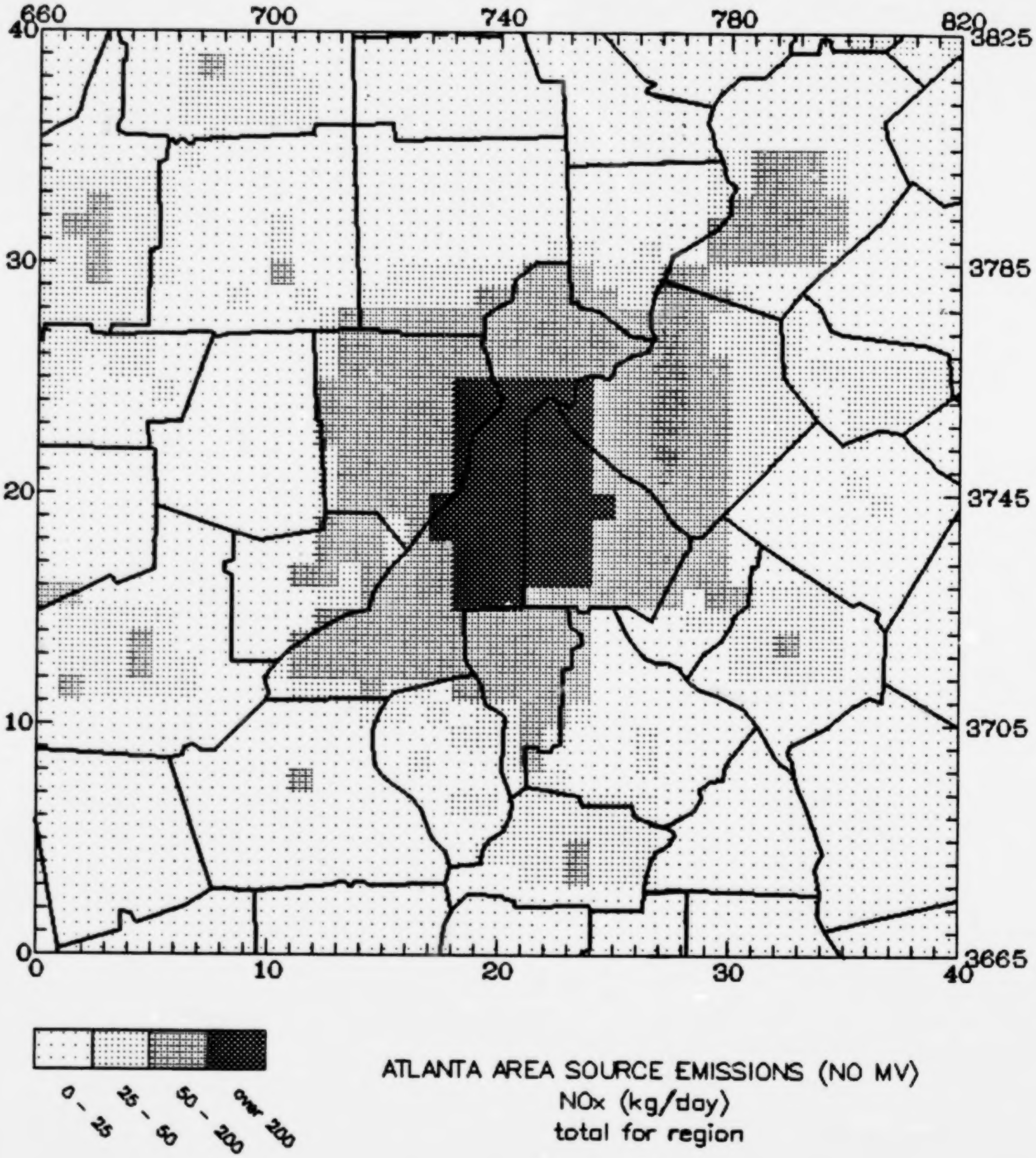
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
0 - 50
50 - 150
150 - 300
over 300

ATLANTA MOTOR VEHICLE EMISSIONS
NOx (kg/day)
Limited Access Roads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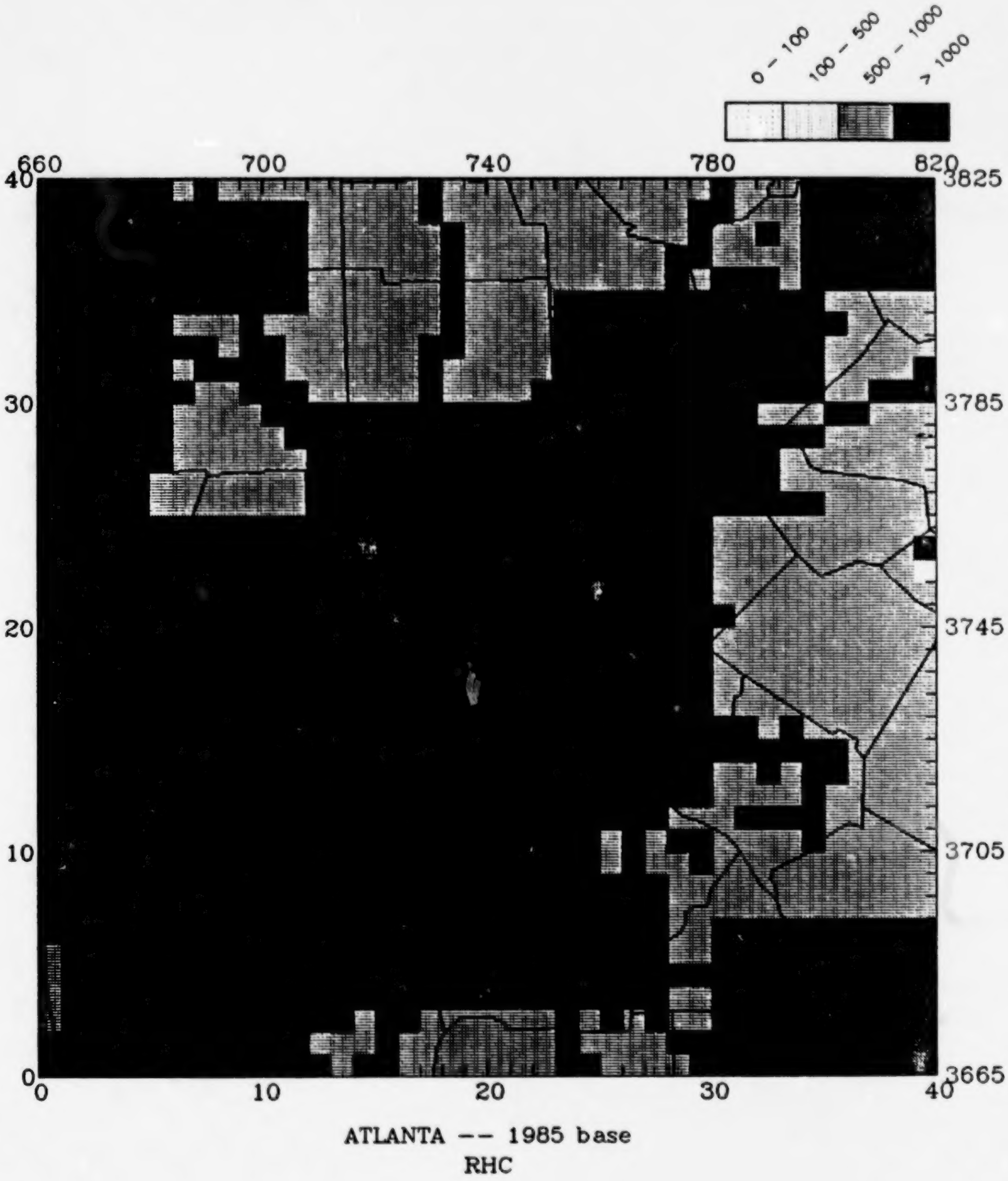
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
0 - 25
25 - 50
50 - 200
over 200

ATLANTA AREA SOURCE EMISSIONS (NO MV)
NOx (kg/day)
total for region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100 - 500
500 - 1000
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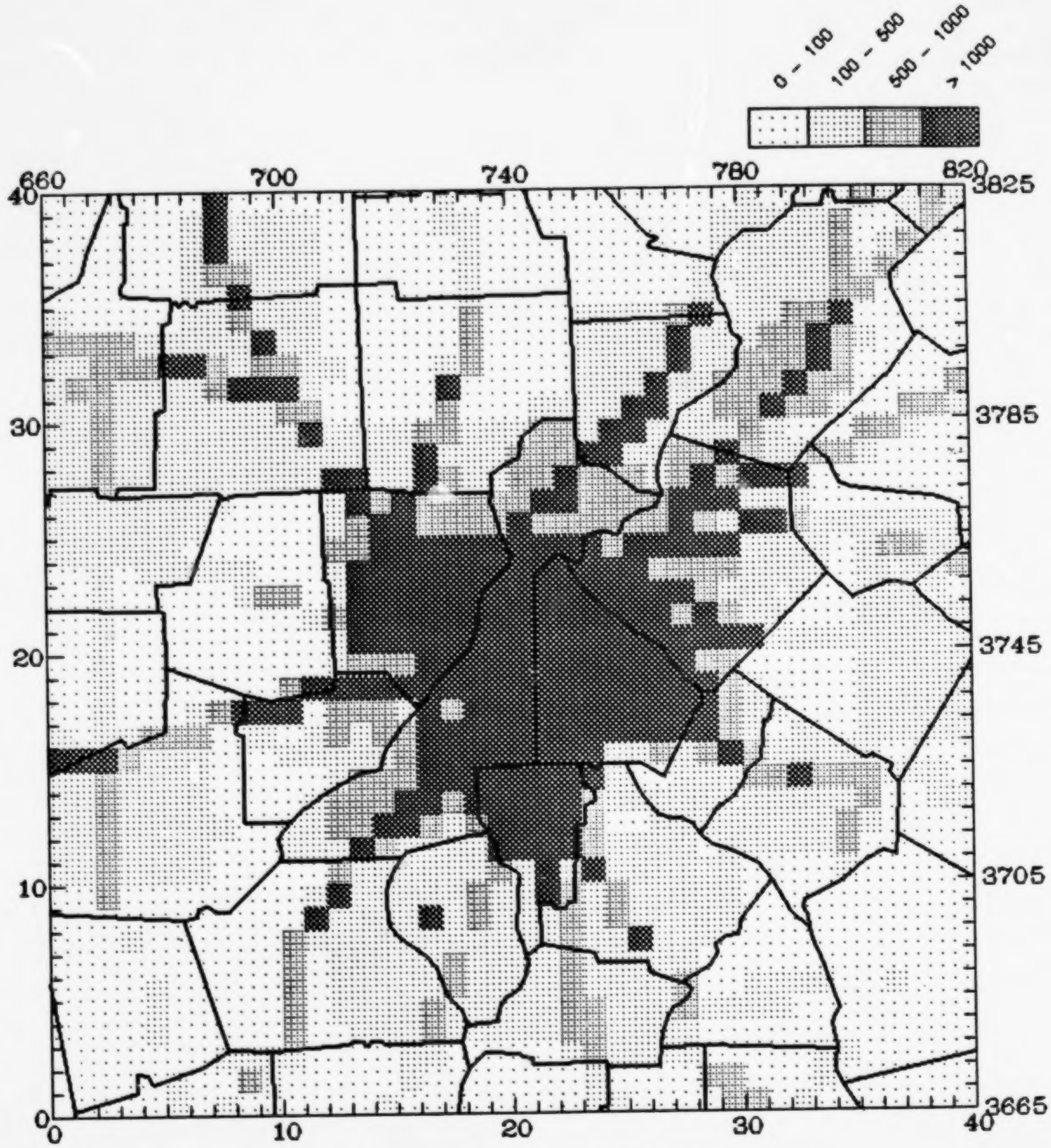
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
ATLANTA -- 1985 base
RHC

Anthropogenic area source and low-level point source plus biogenic VOC emissions (kg/day).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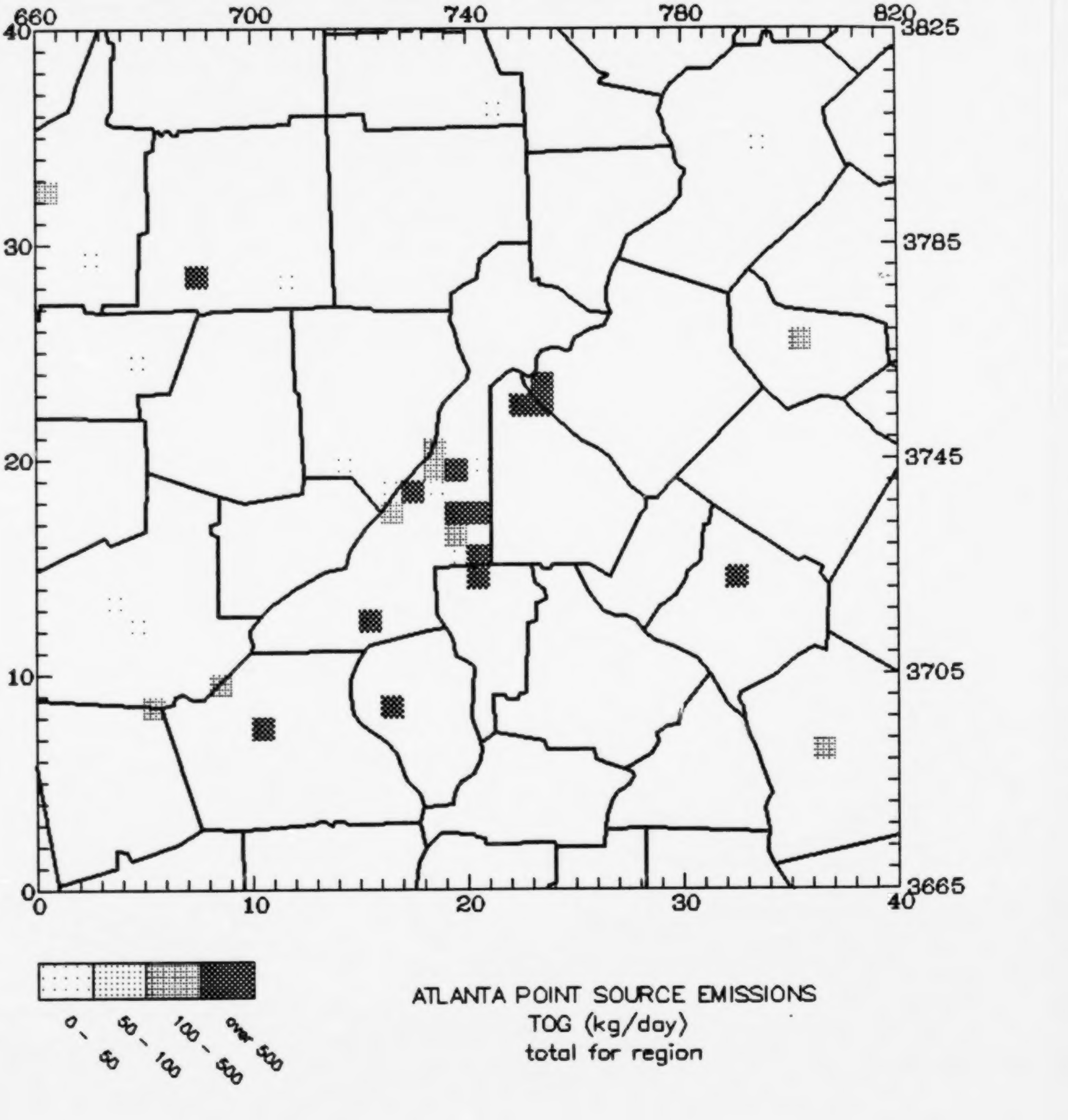
500 - 1000
> 1000
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

ATLANTA -- 1985 base -- anthropogenic only
RHC
(Kg/day)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700
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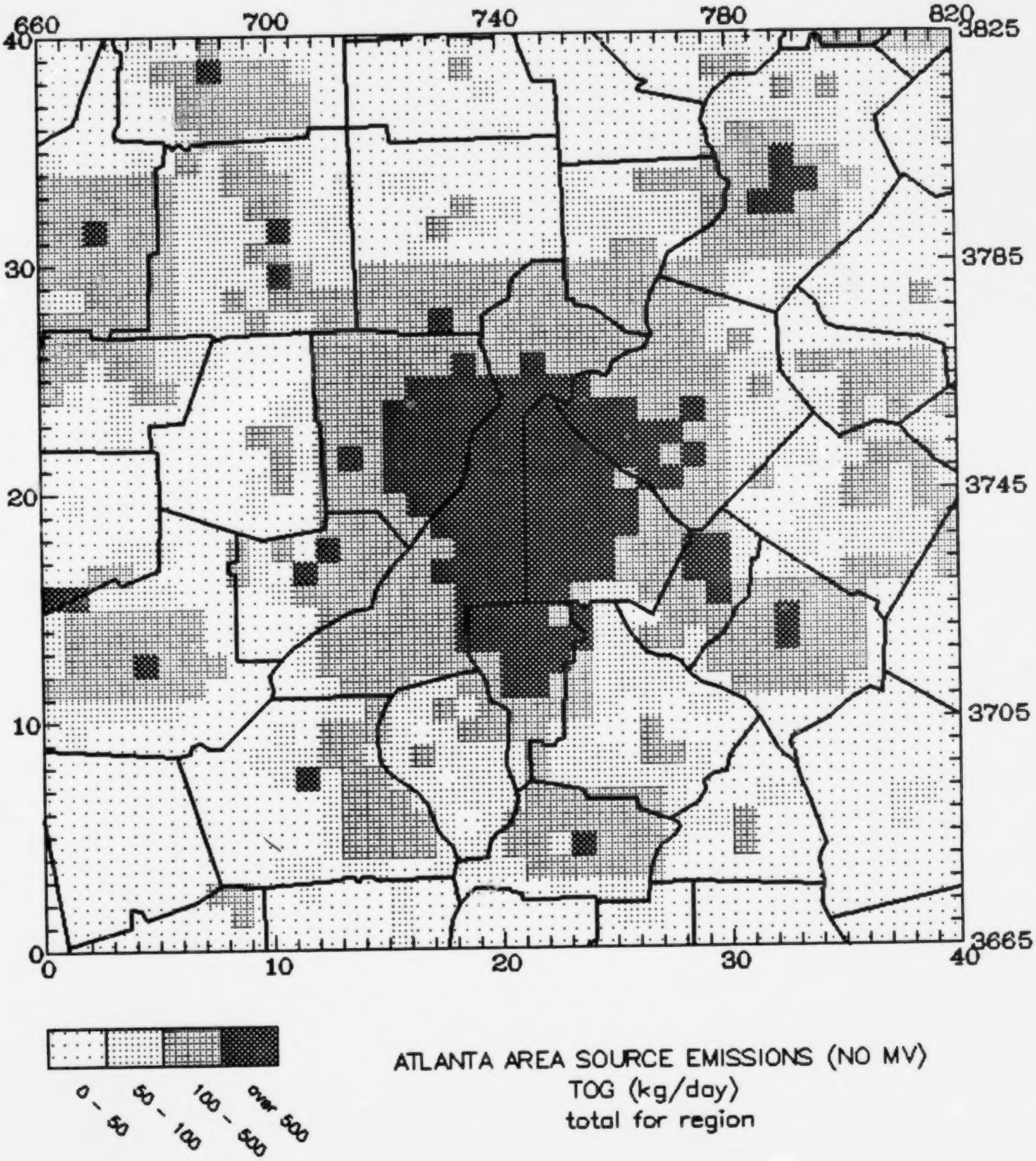
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
0 - 50
50 - 100
100 - 500
over 500

ATLANTA POINT SOURCE EMISSIONS
TOG (kg/day)
total for region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820
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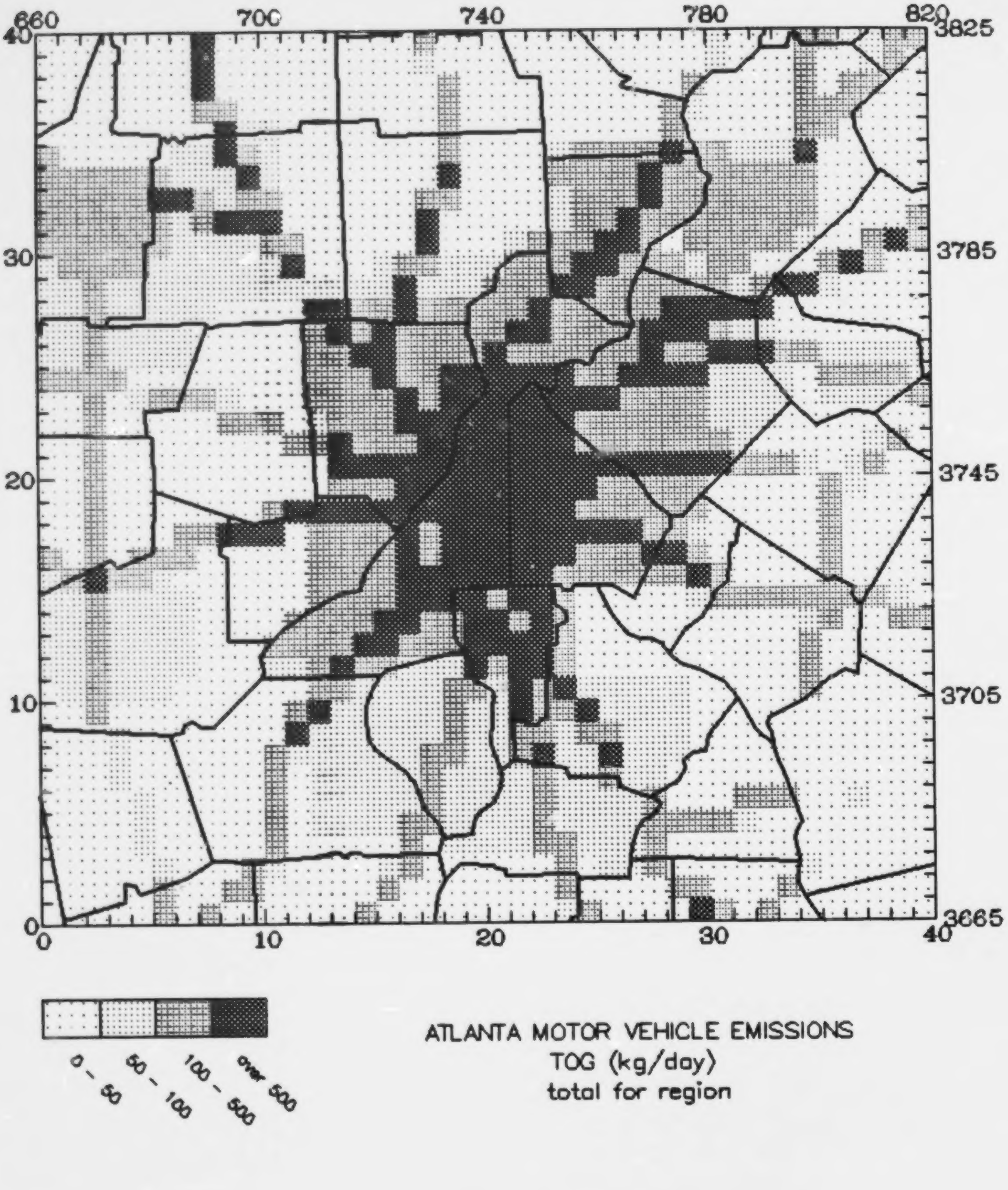
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
0 - 50
50 - 100
100 - 500
over 500

ATLANTA AREA SOURCE EMISSIONS (NO MV)
TOG (kg/day)
total for region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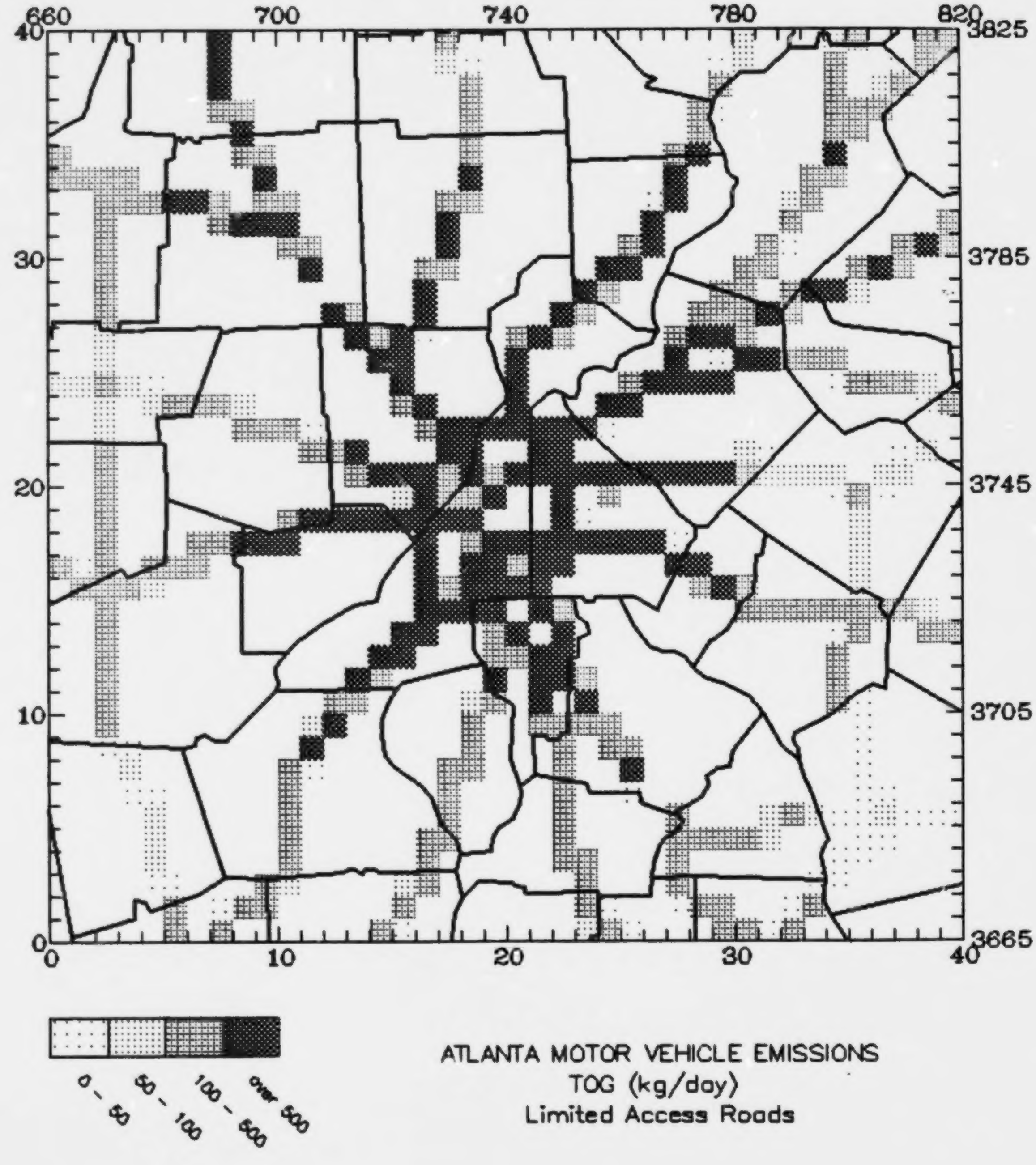
700
740
780
820
3825
3785
3745
3705
3665
0
10
20
30
40
0 - 50
50 - 100
100 - 500
over 500

ATLANTA MOTOR VEHICLE EMISSIONS
TOG (kg/day)
total for region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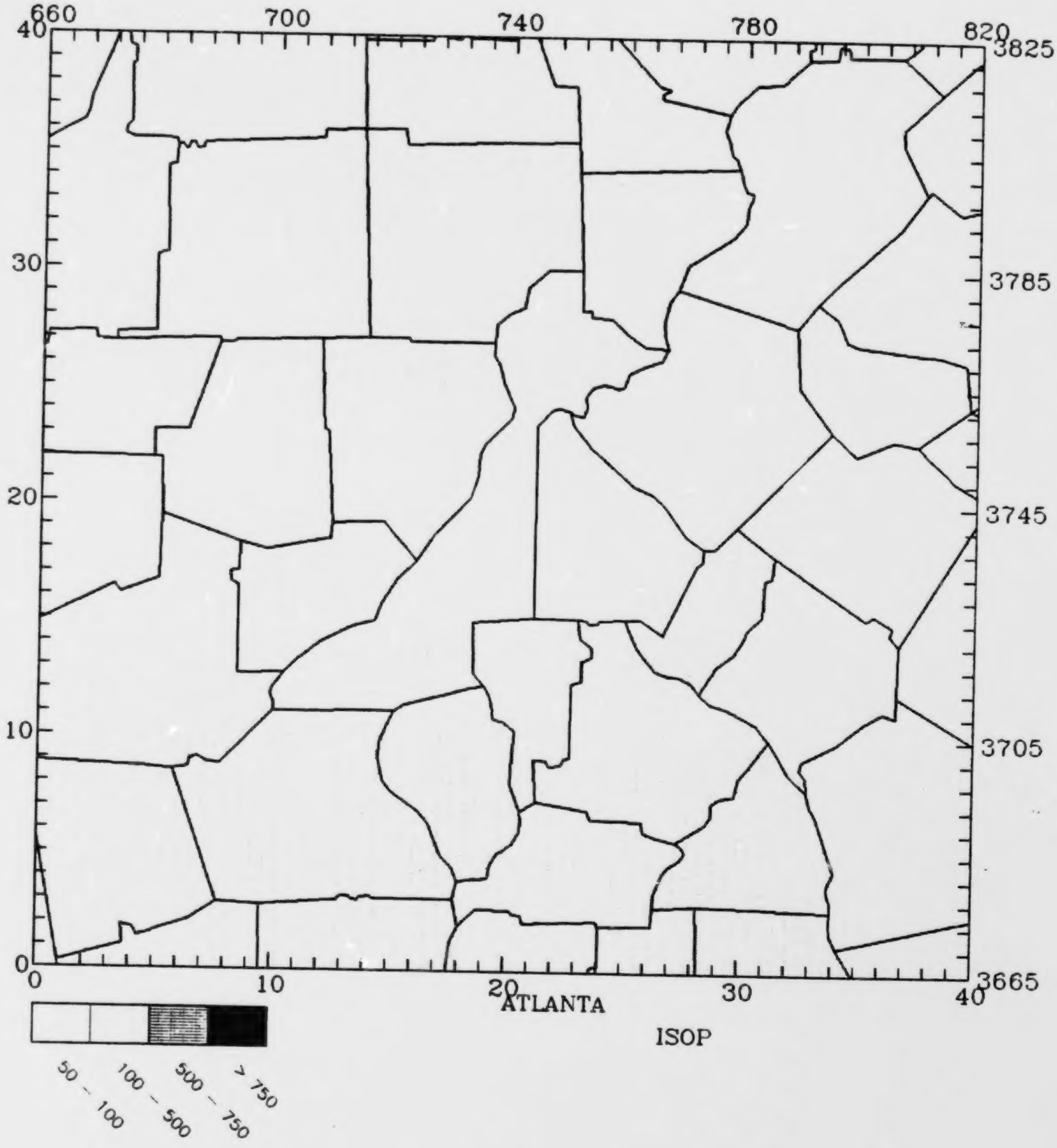
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
0 - 50
50 - 100
100 - 500
over 500

ATLANTA MOTOR VEHICLE EMISSIONS
TOG (kg/day)
Limited Access Roads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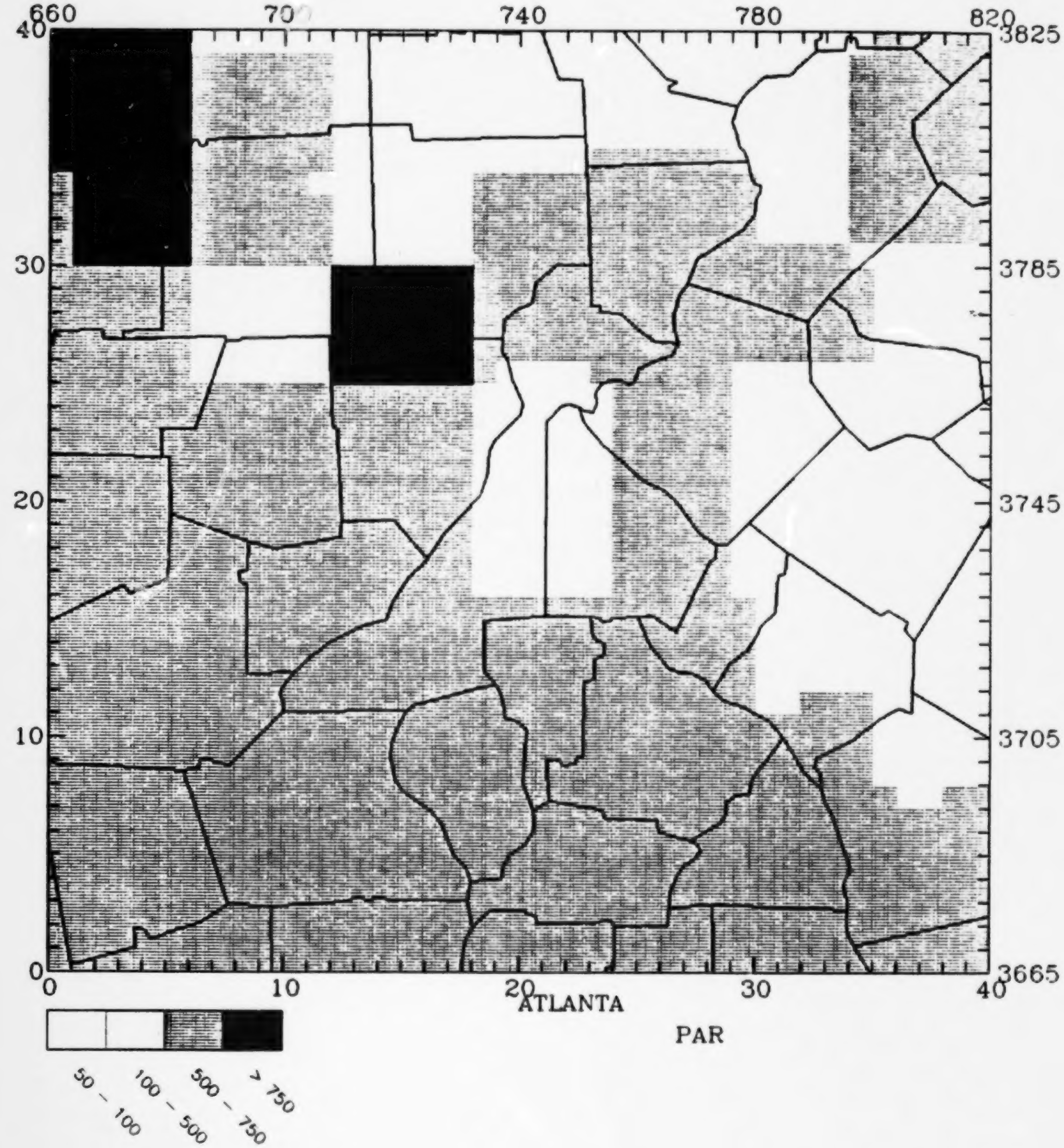
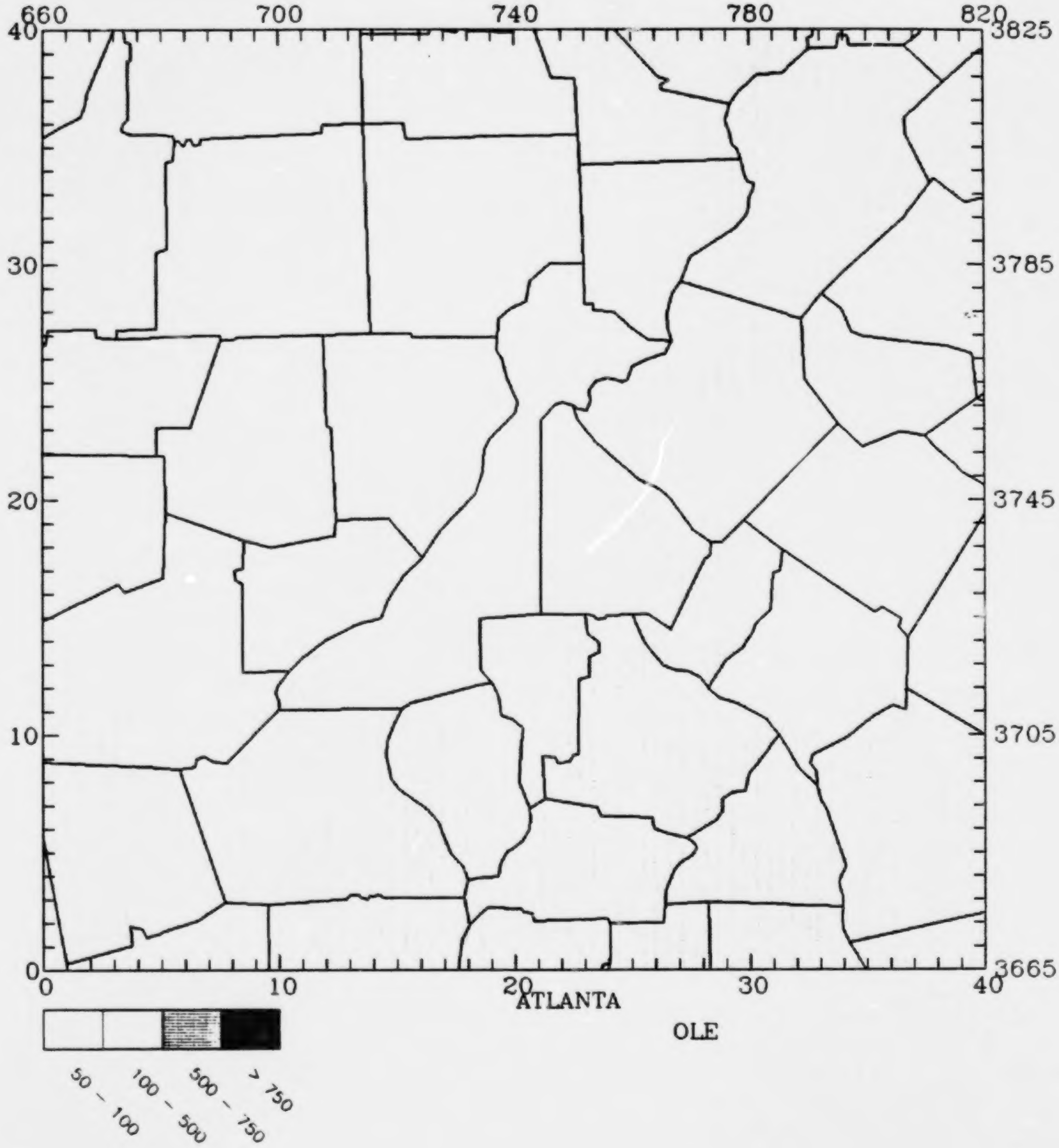
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
ATLANTA
ISOP
50 - 100
100 - 500
500 - 750
> 750

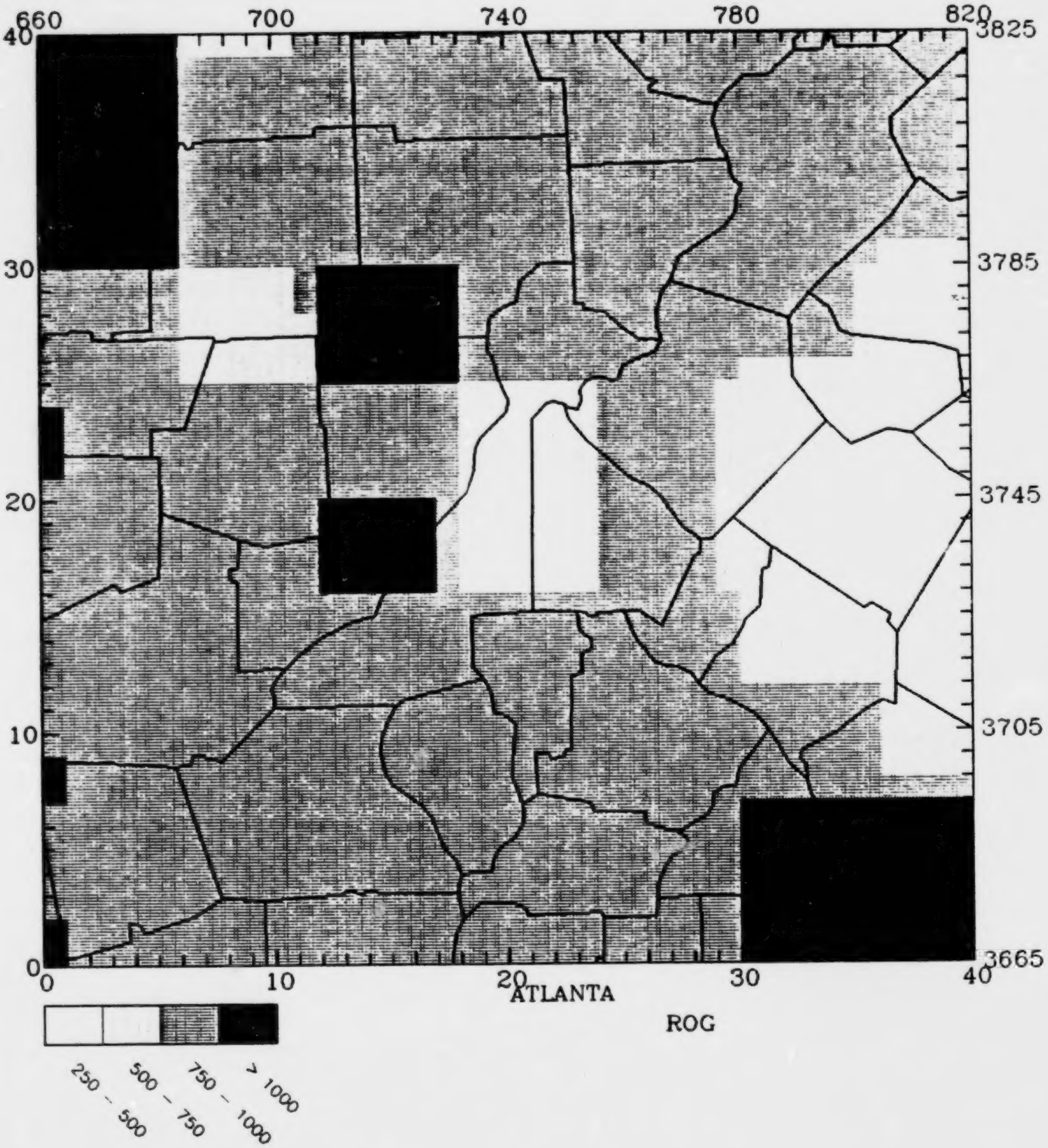
Total biogenic ISOP emissions (kg/day) for the Atlanta UAM modeling domain


660
700
740
780
820
3825
3785
3745
3705
3665
0
10
20
30
40
ATLANTA
PAR
50 – 100
100 – 500
500 – 750
> 750

Total biogenic PAR emissions (kg/day) for the Atlanta UAM modeling domain


660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
ATLANTA
OLE
50 – 100
100 – 500
500 – 750
> 750

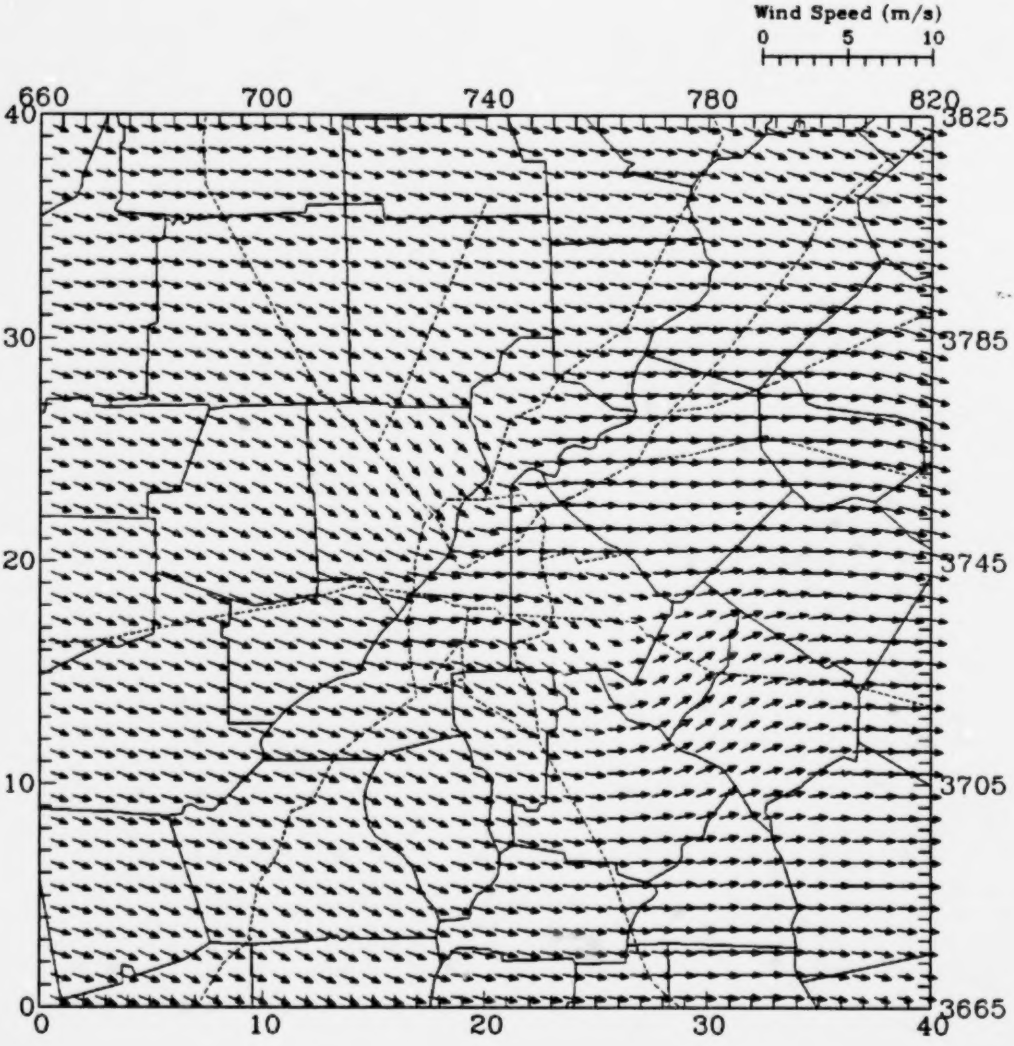
Total biogenic OLE emissions (kg/day) for the Atlanta UAM modeling domain


660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40
ATLANTA
ROG
250 - 500
500 - 750
750 - 1000
> 1000

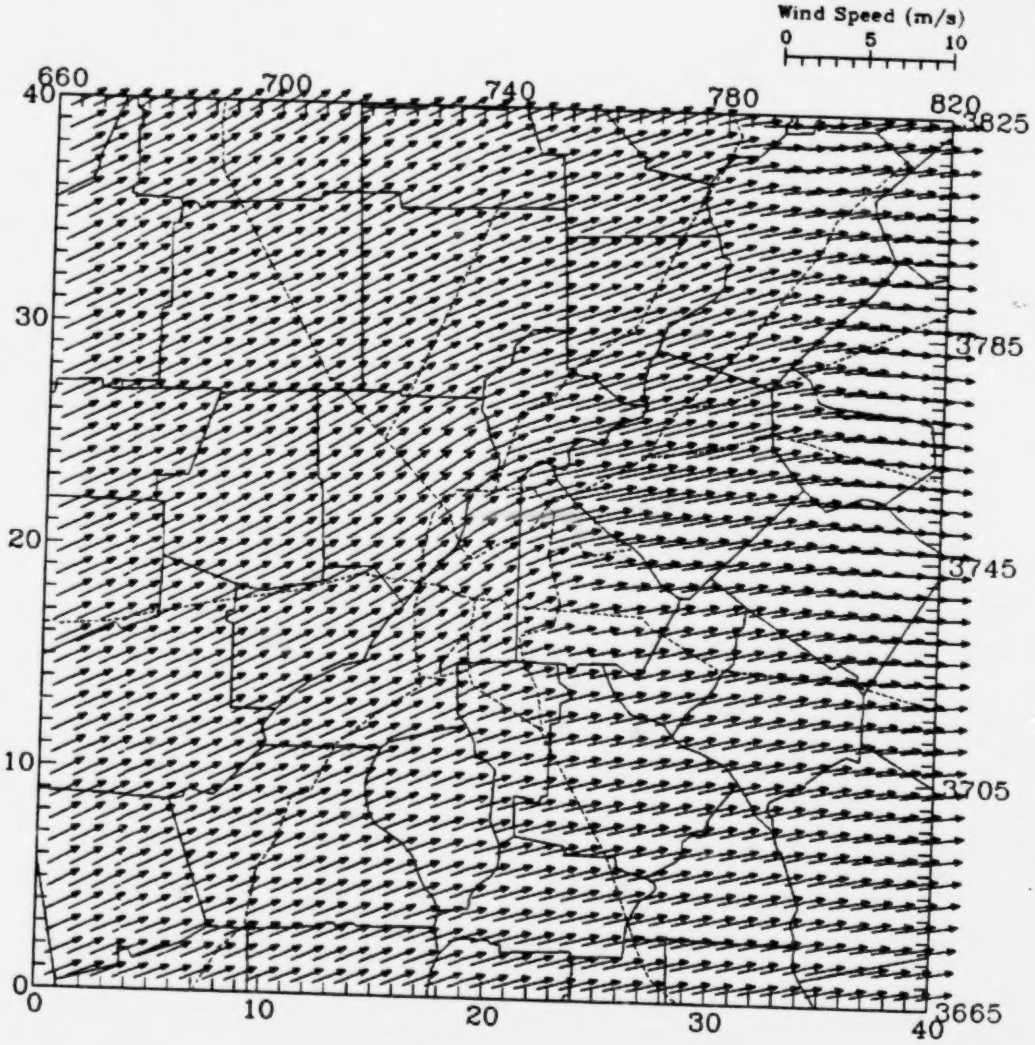
Total biogenic VOC emissions (kg/day) for the Atlanta UAM modeling domain

Appendix B

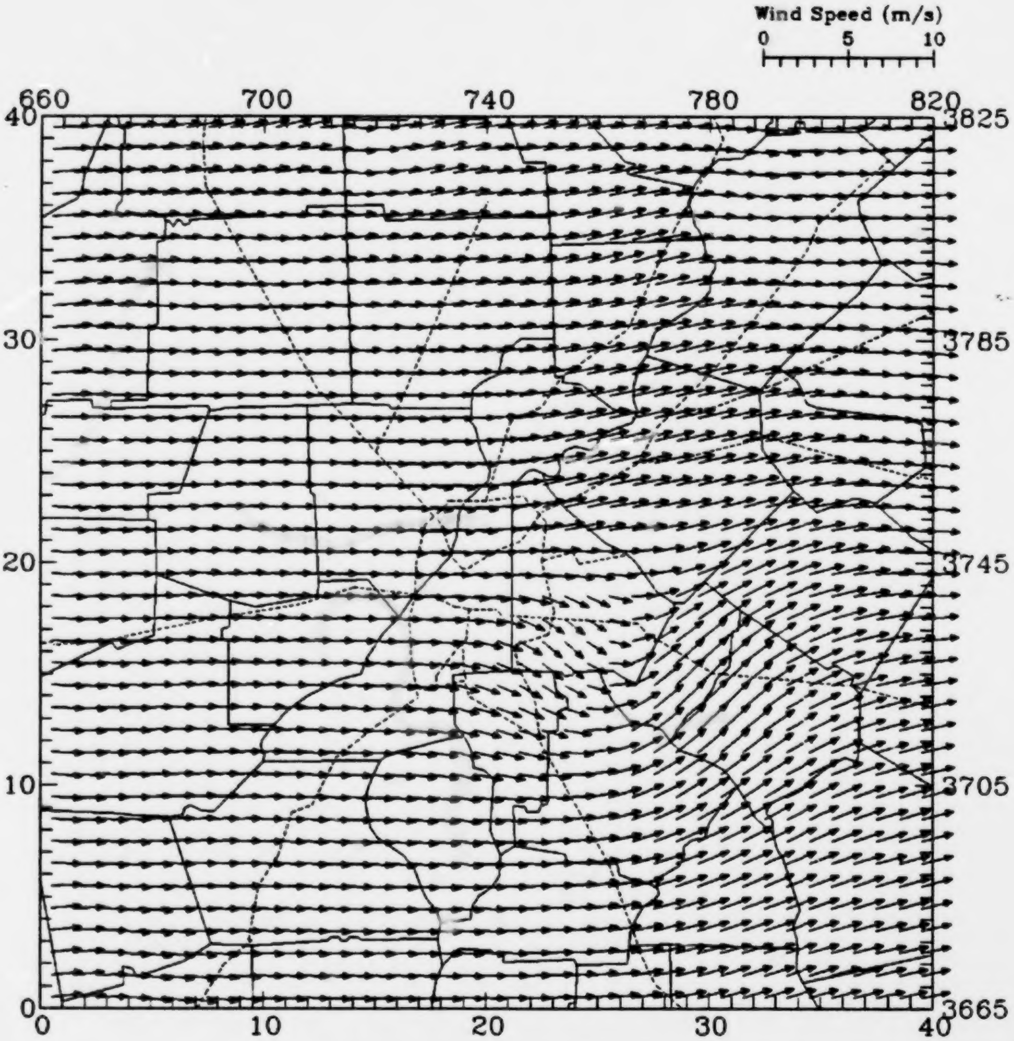
HOURLY WIND FIELDS FOR UAM LAYER 1 USED IN DIAGNOSTIC RUN 1


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

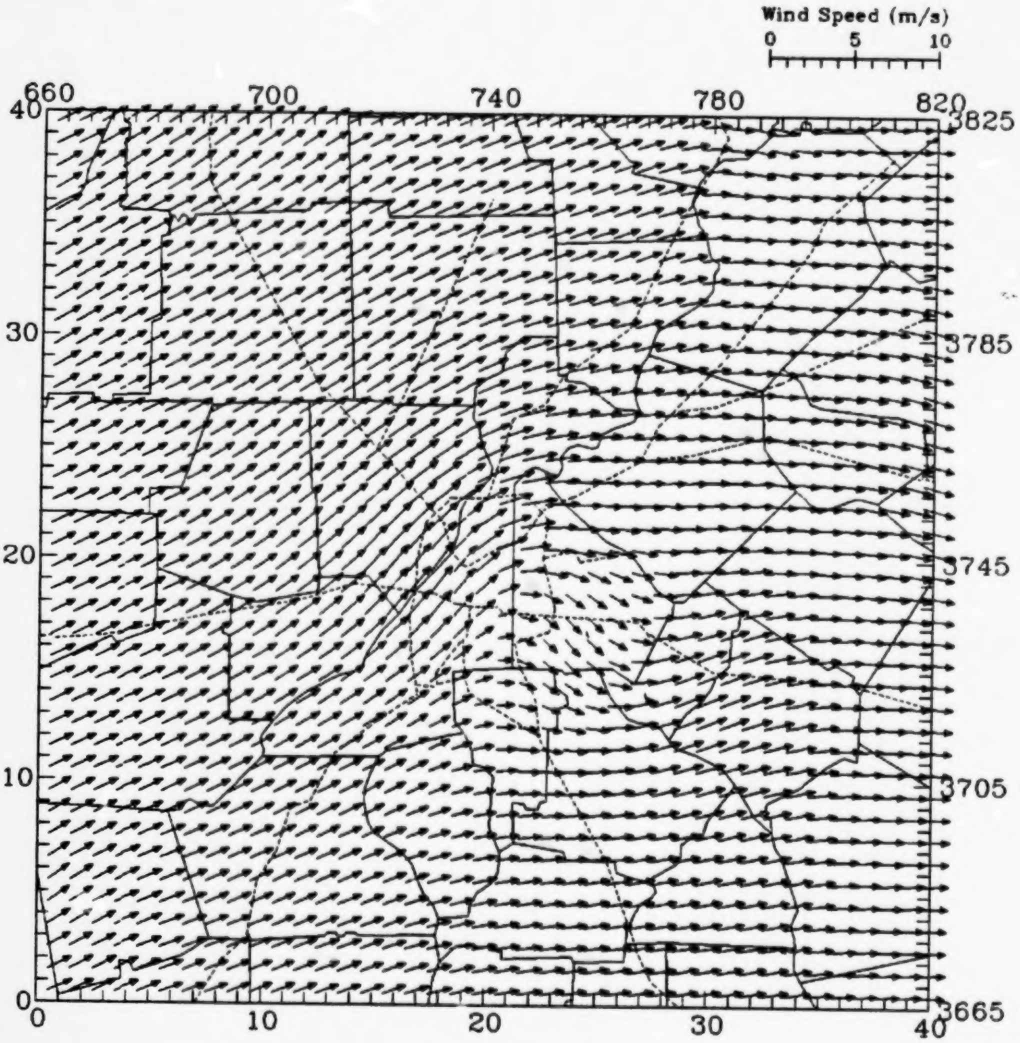
Atlanta PLANR Winds
Layer 1 at hour 10 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
40
30
20
10
0
0
10
20
30
40
3825
3785
3745
3705
3665

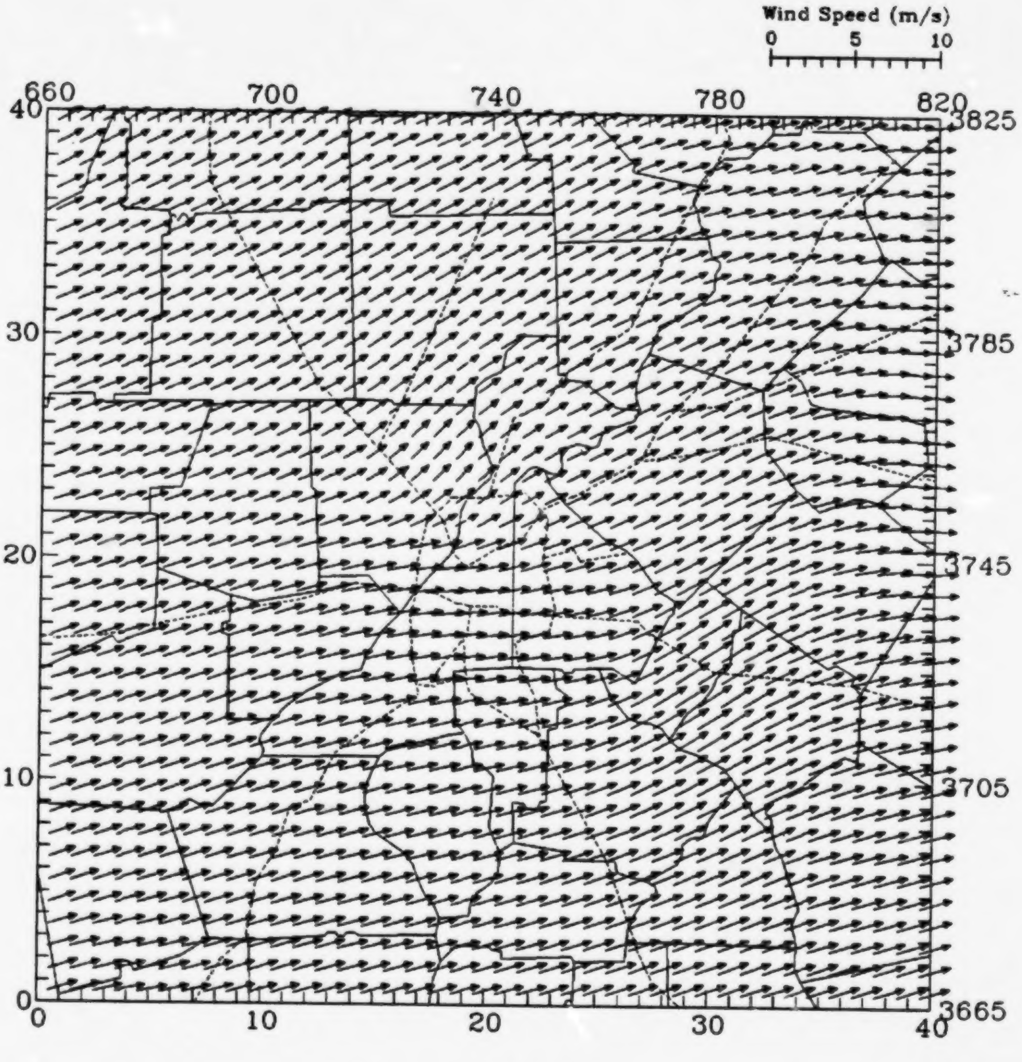
Atlanta PLANR Winds
Layer 1 at hour 11 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

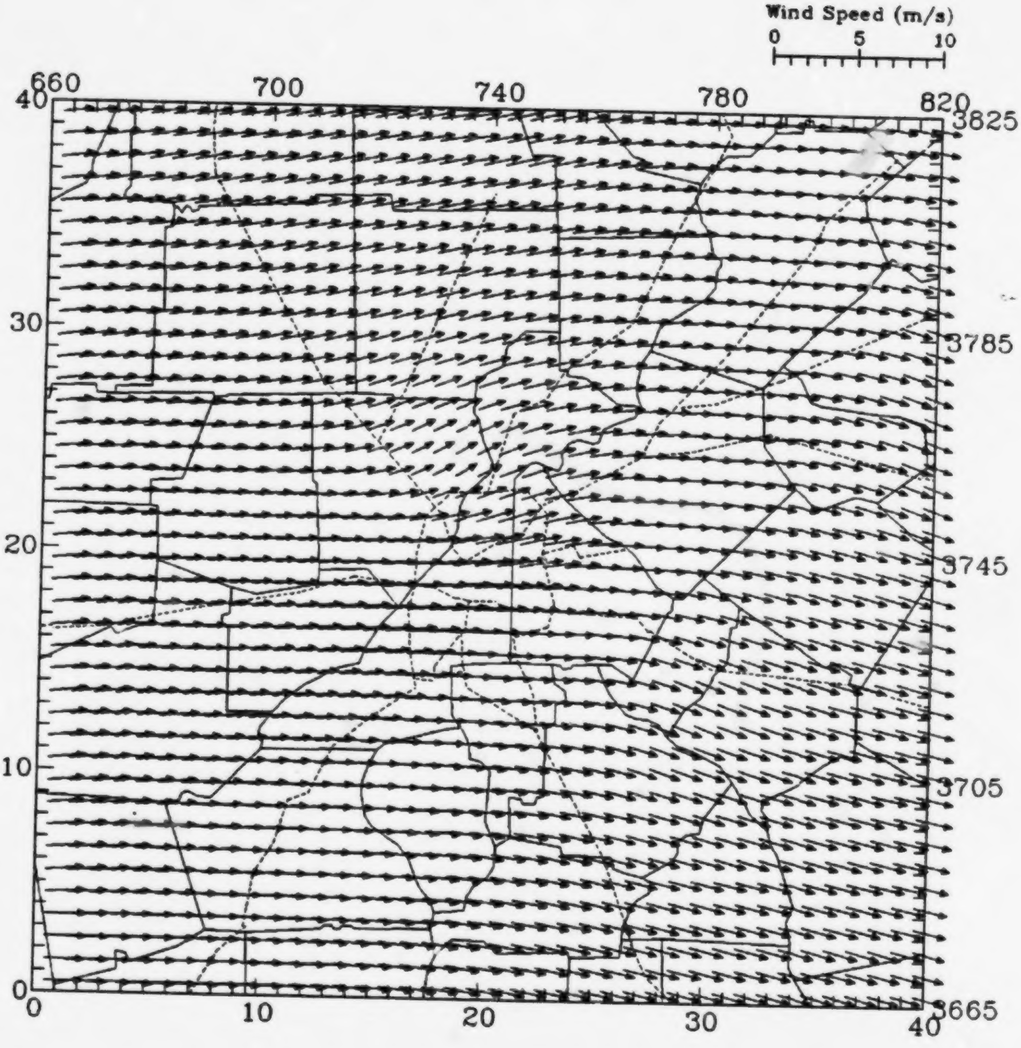
Atlanta PLANR Winds
Layer 1 at hour 12 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
40
30
20
10
0
0
10
20
30
40
3825
3785
3745
3705
3665

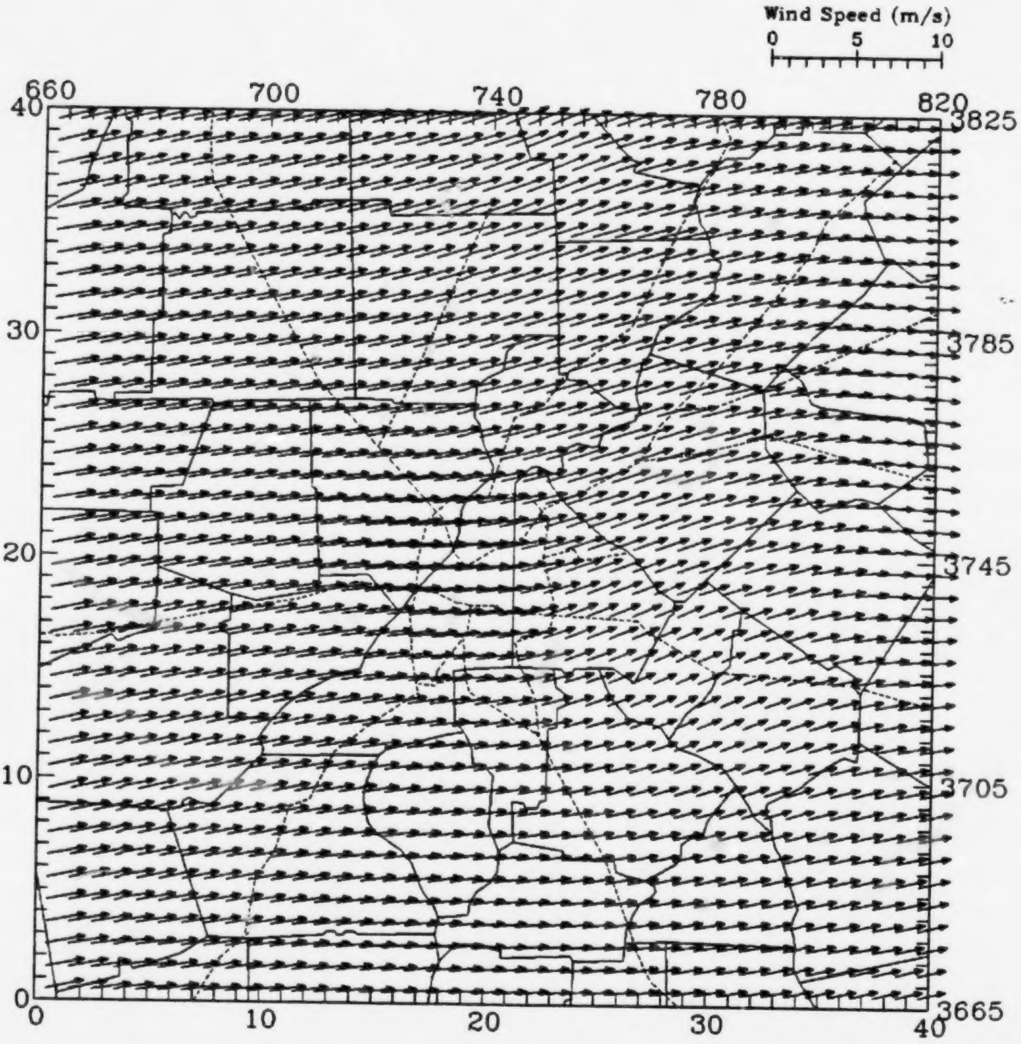
Atlanta PLANR Winds
Layer 1 at hour 13 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

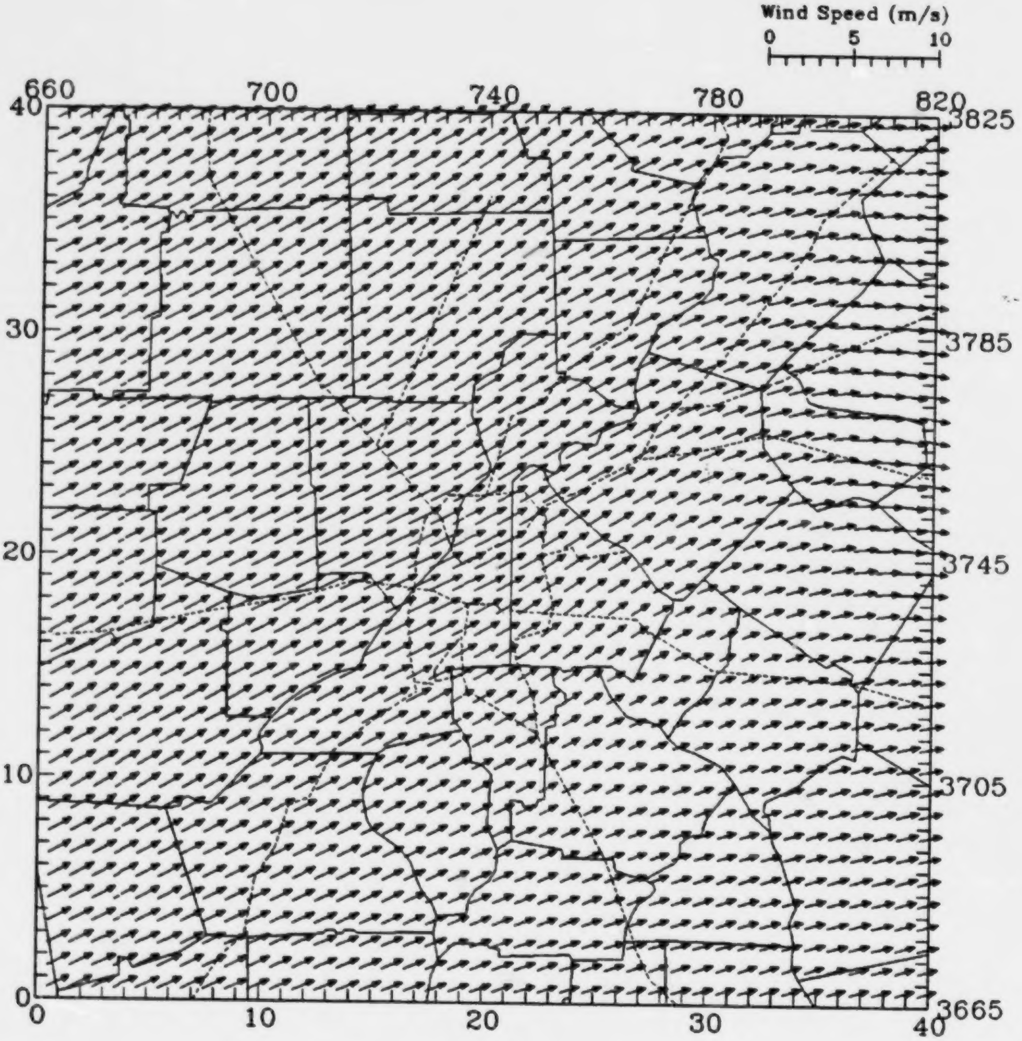
Atlanta PLANR Winds
Layer 1 at hour 14 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

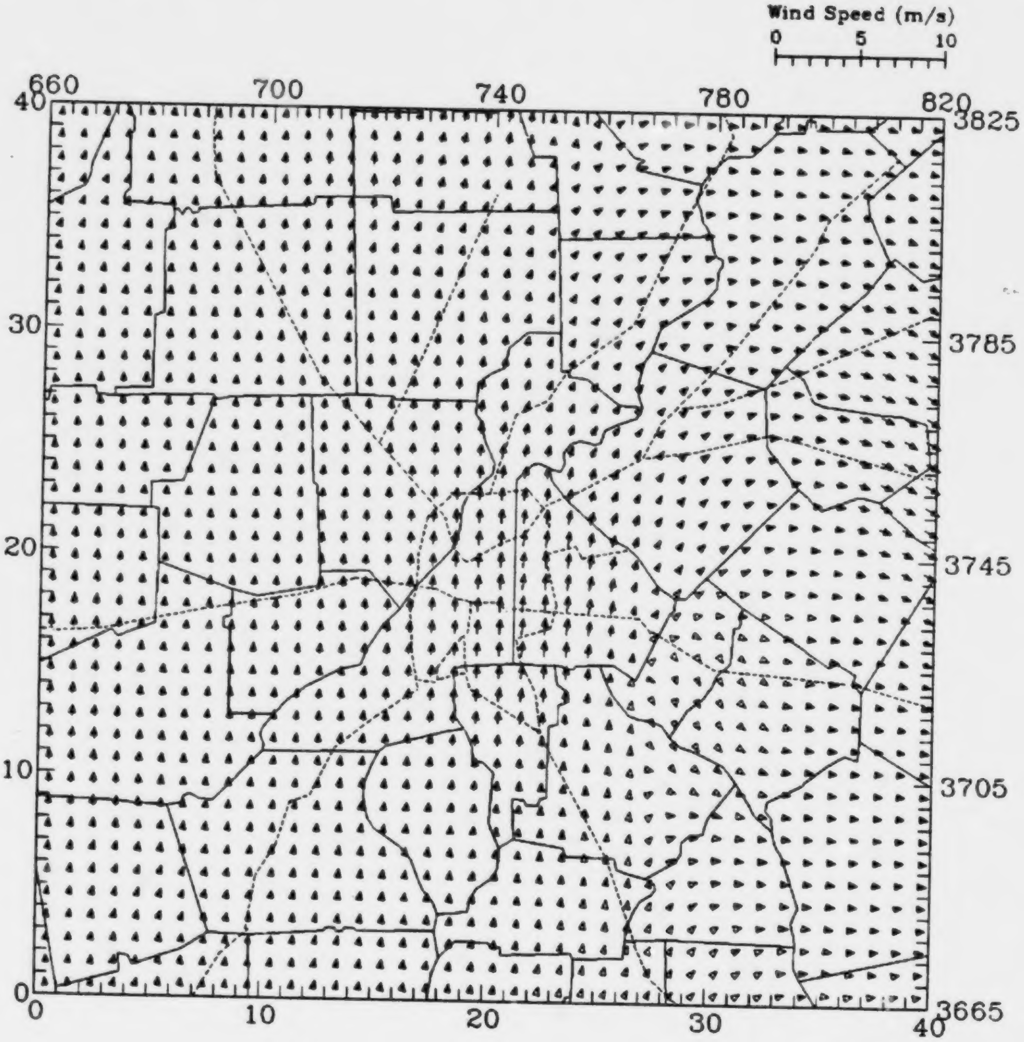
Atlanta PLANR Winds
Layer 1 at hour 15 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
0
10
20
30
40

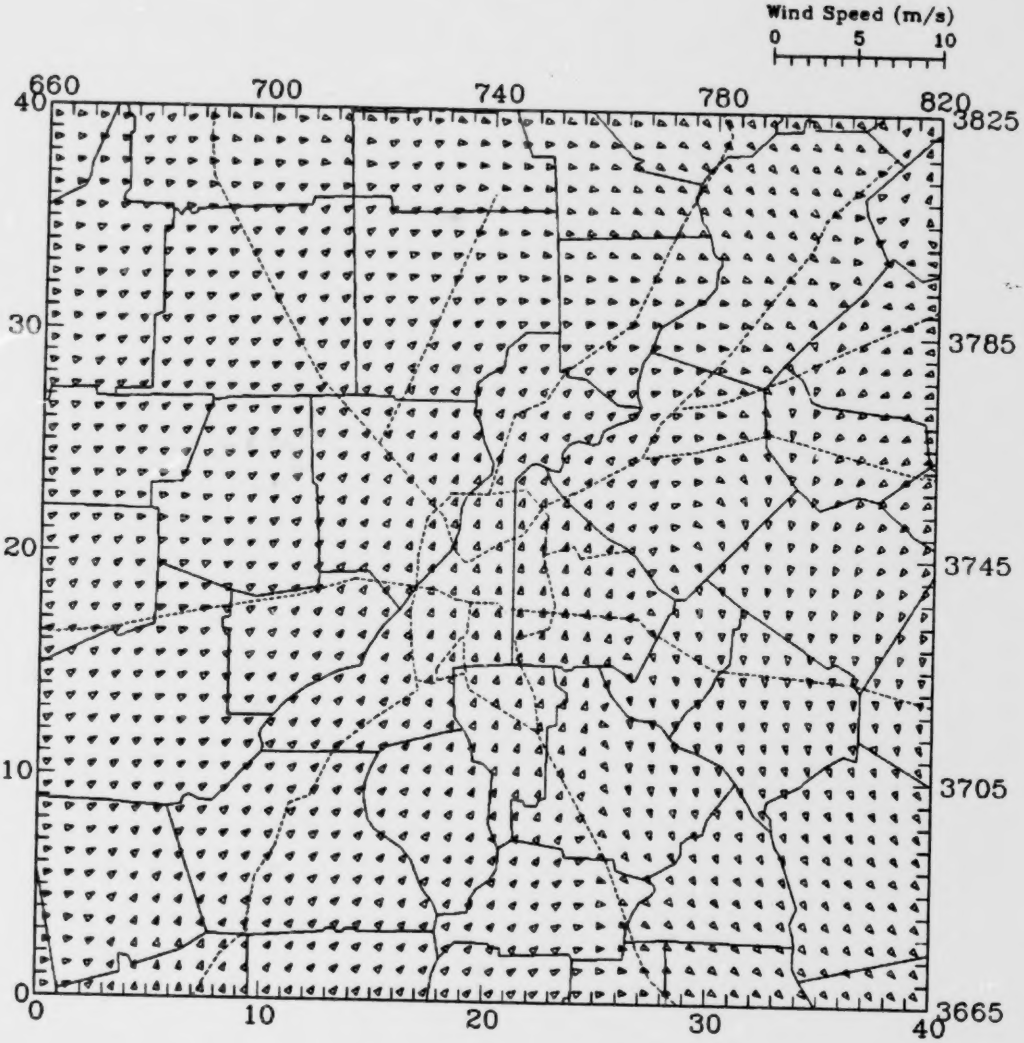
Atlanta PLANR Winds
Layer 1 at hour 16 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
0
10
20
30
40

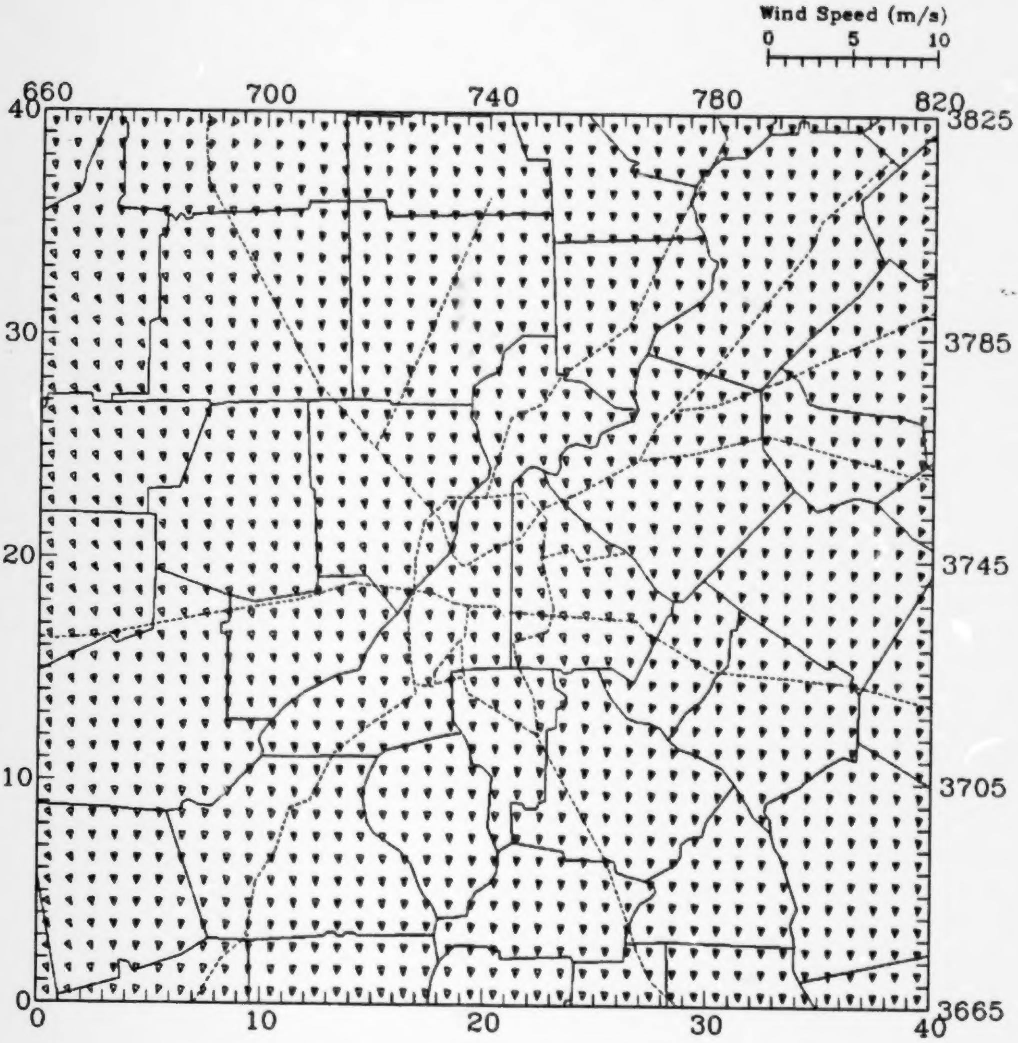
Atlanta PLANR Winds
Layer 1 at hour 17 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

Atlanta PLANR Winds
Layer 1 at hour 18 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

Atlanta PLANR Winds
Layer 1 at hour 19 on 84156

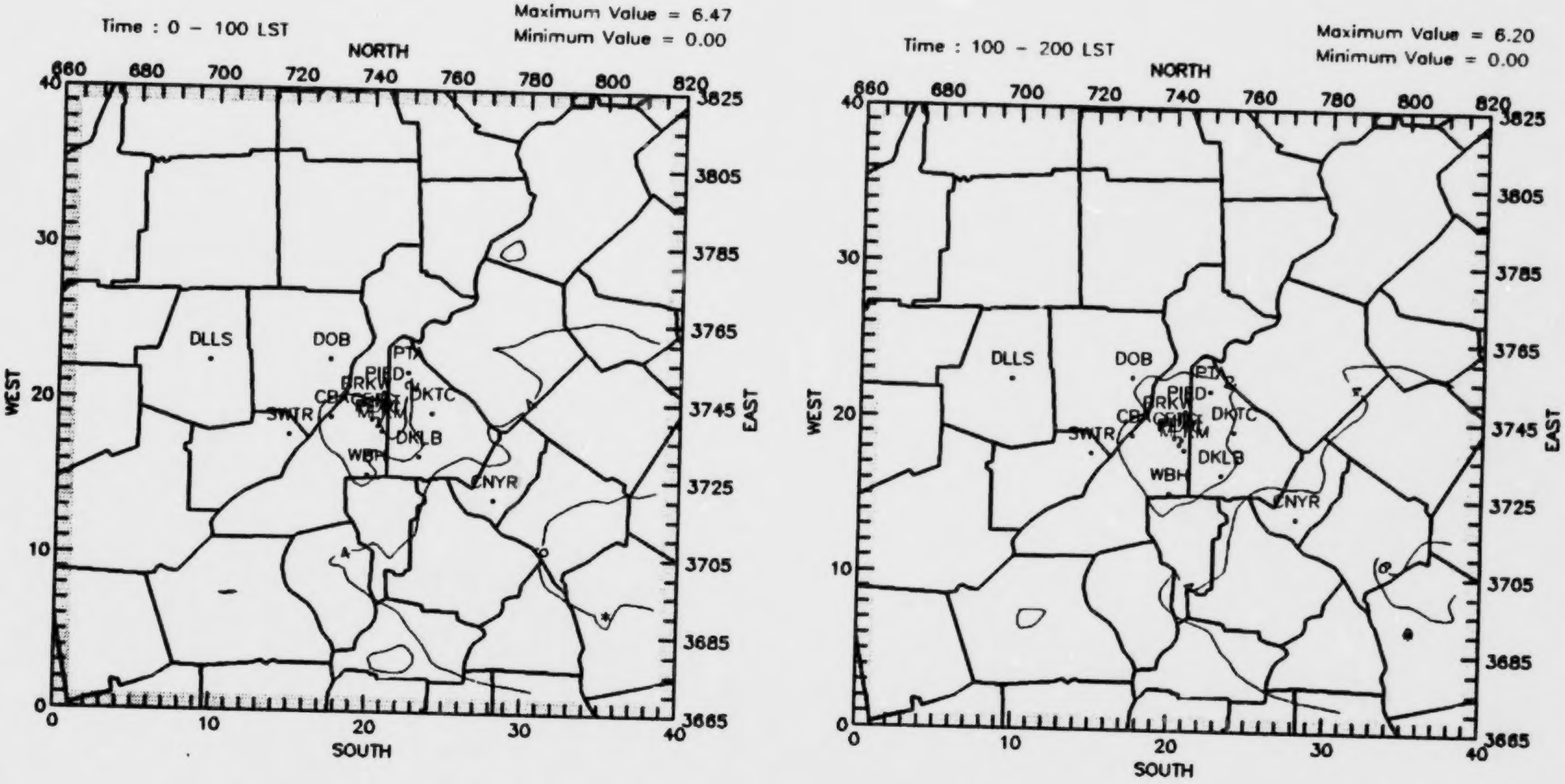

Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

Atlanta PLANR Winds
Layer 1 at hour 20 on 84156

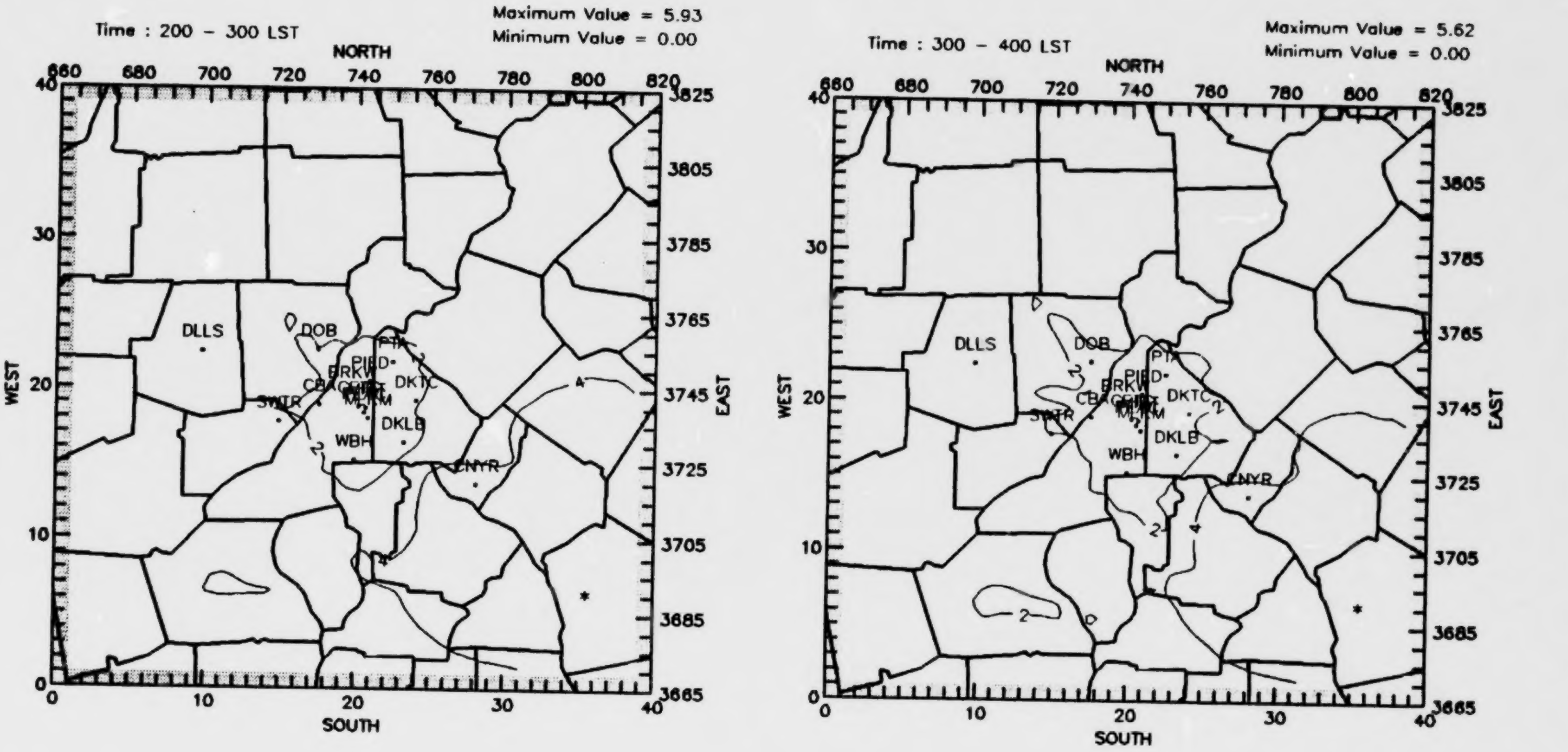
[illegible]

Appendix C

HOURLY PREDICTED OZONE CONCENTRATIONS (pphm) FOR DIAGNOSTIC RUN 1


Time : 0 - 100 LST
Maximum Value = 6.47
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
SWTR
PIED
BRKW
PTX
DKTC
DKLB
WBH
CNYR
Time : 100 - 200 LST
Maximum Value = 6.20
Minimum Value = 0.00

Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)



Time : 200 - 300 LST

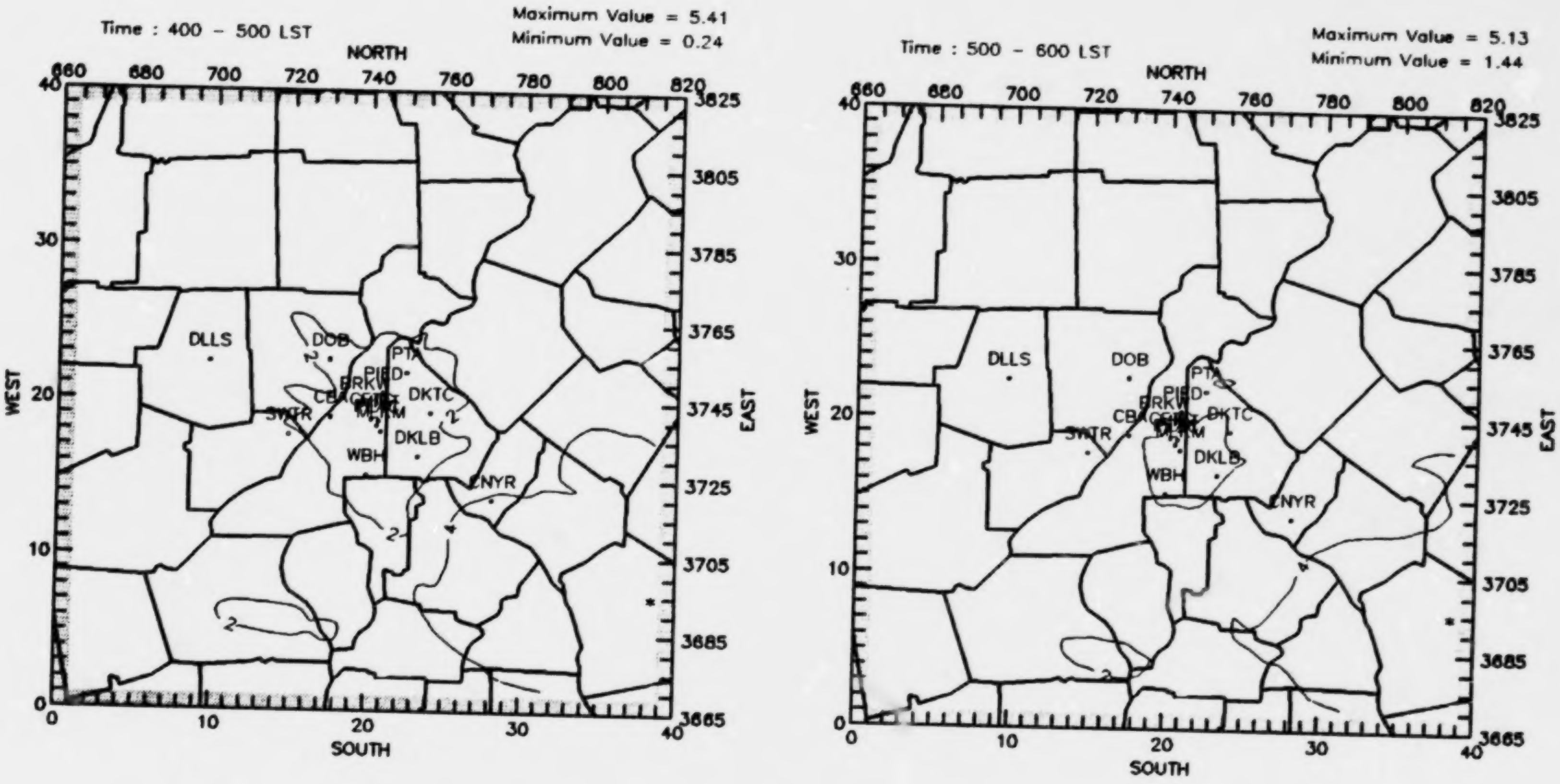
Maximum Value = 5.93
Minimum Value = 0.00

Time : 300 - 400 LST

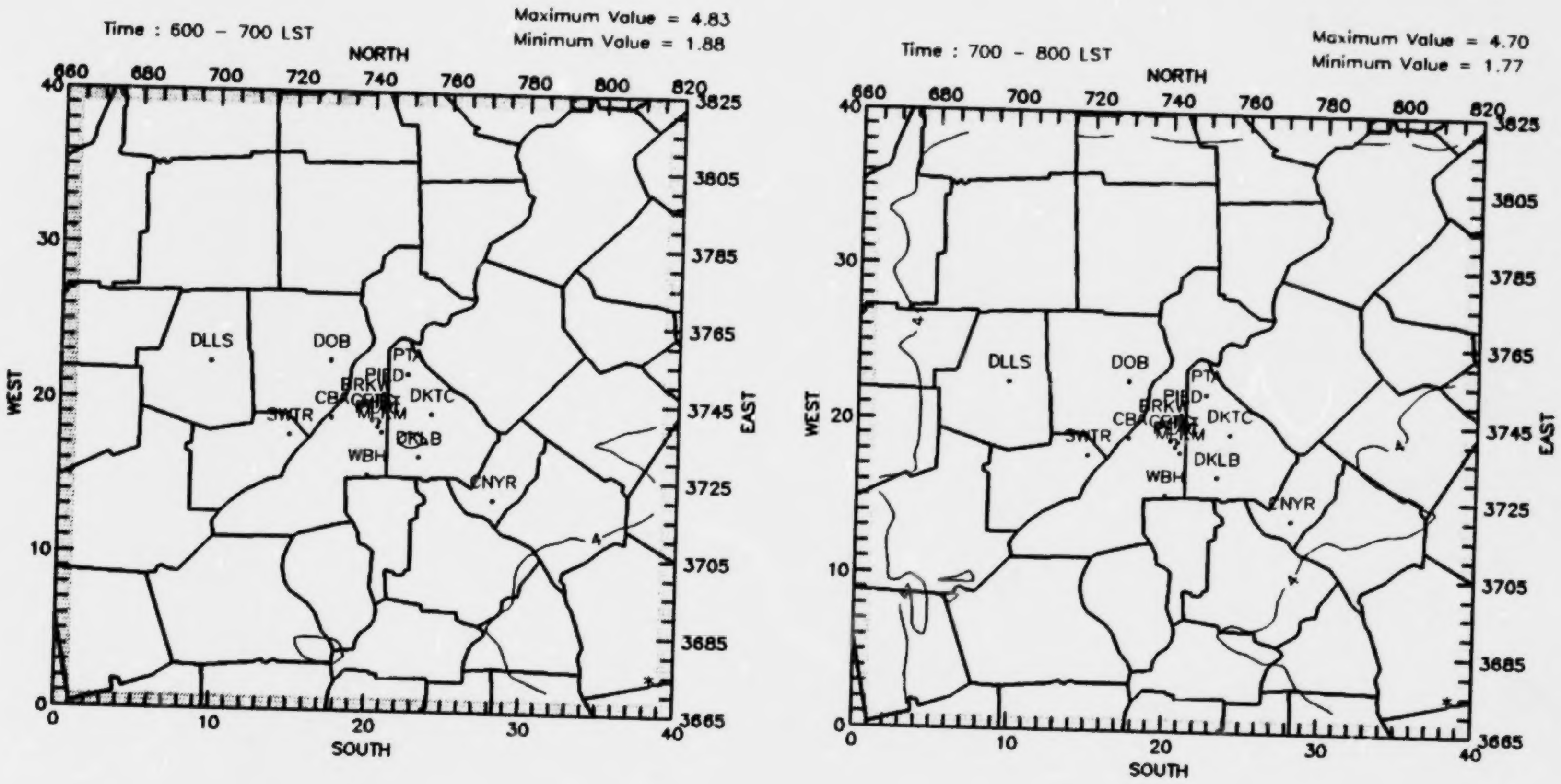
Maximum Value = 5.62
Minimum Value = 0.00

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PIED
BRKW
CBAC
PTA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
2
4
0

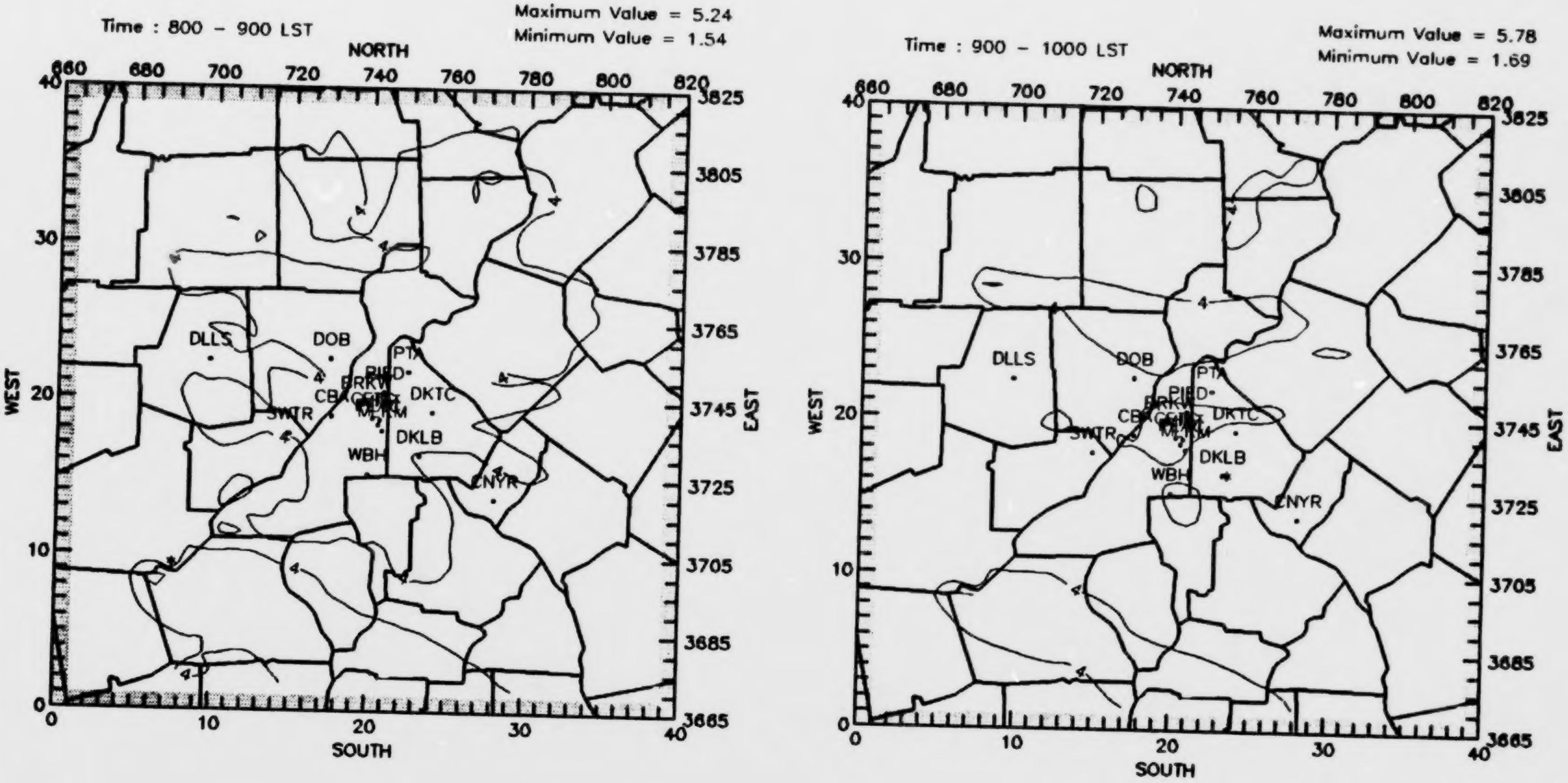
Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)


Time : 400 - 500 LST
Maximum Value = 5.41
Minimum Value = 0.24
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PT
PIRD-
BRKW
CBA
DKTC
SWTR
MTM
DKLB
WBH
CNYR
2
4
Time : 500 - 600 LST
Maximum Value = 5.13
Minimum Value = 1.44

Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)


Time : 600 - 700 LST
Maximum Value = 4.83
Minimum Value = 1.88
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
DKLB
WBH
CNYR
4
Time : 700 - 800 LST
Maximum Value = 4.70
Minimum Value = 1.77

Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)


Time : 800 - 900 LST

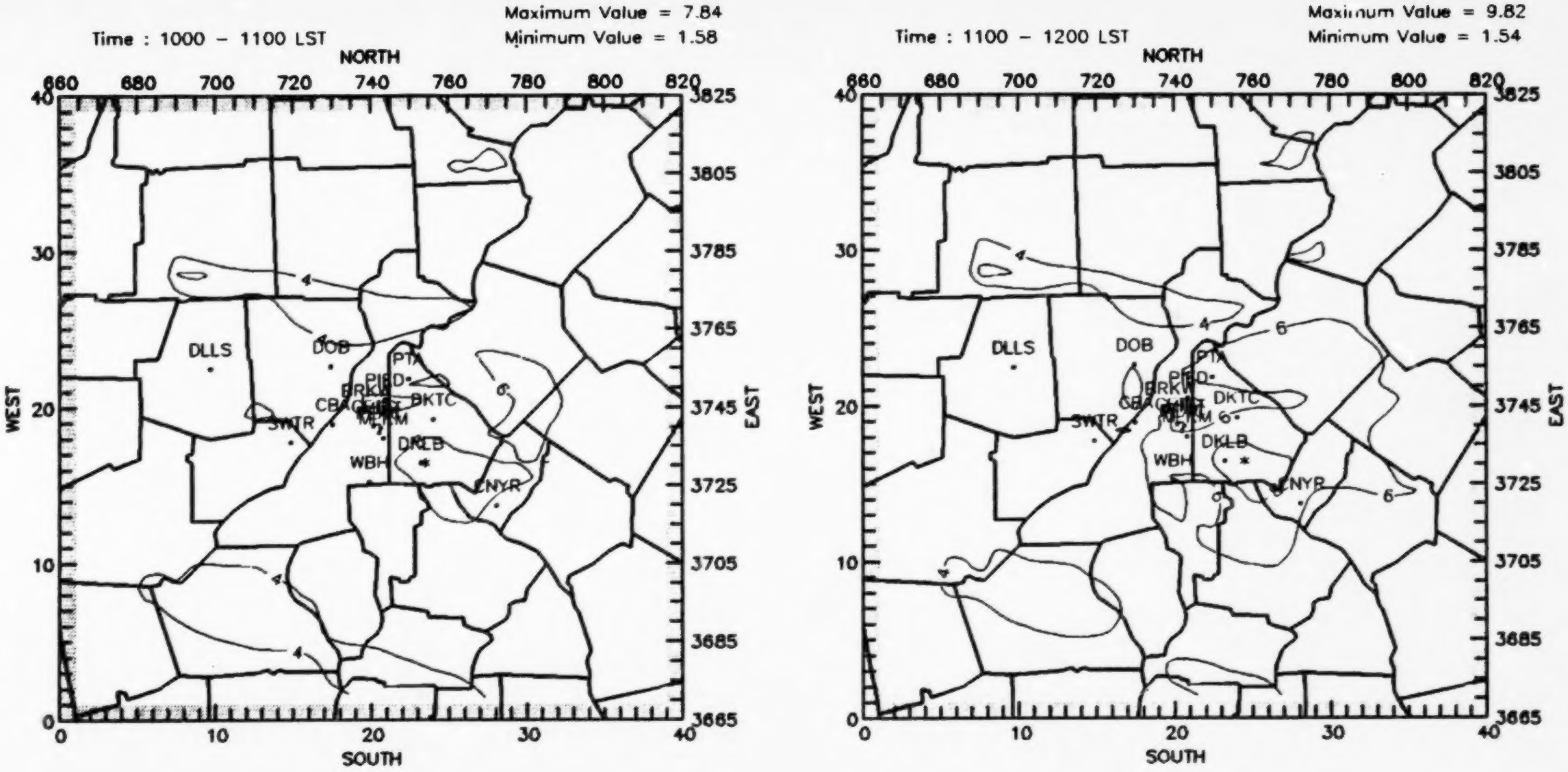
Maximum Value = 5.24
Minimum Value = 1.54

Time : 900 - 1000 LST

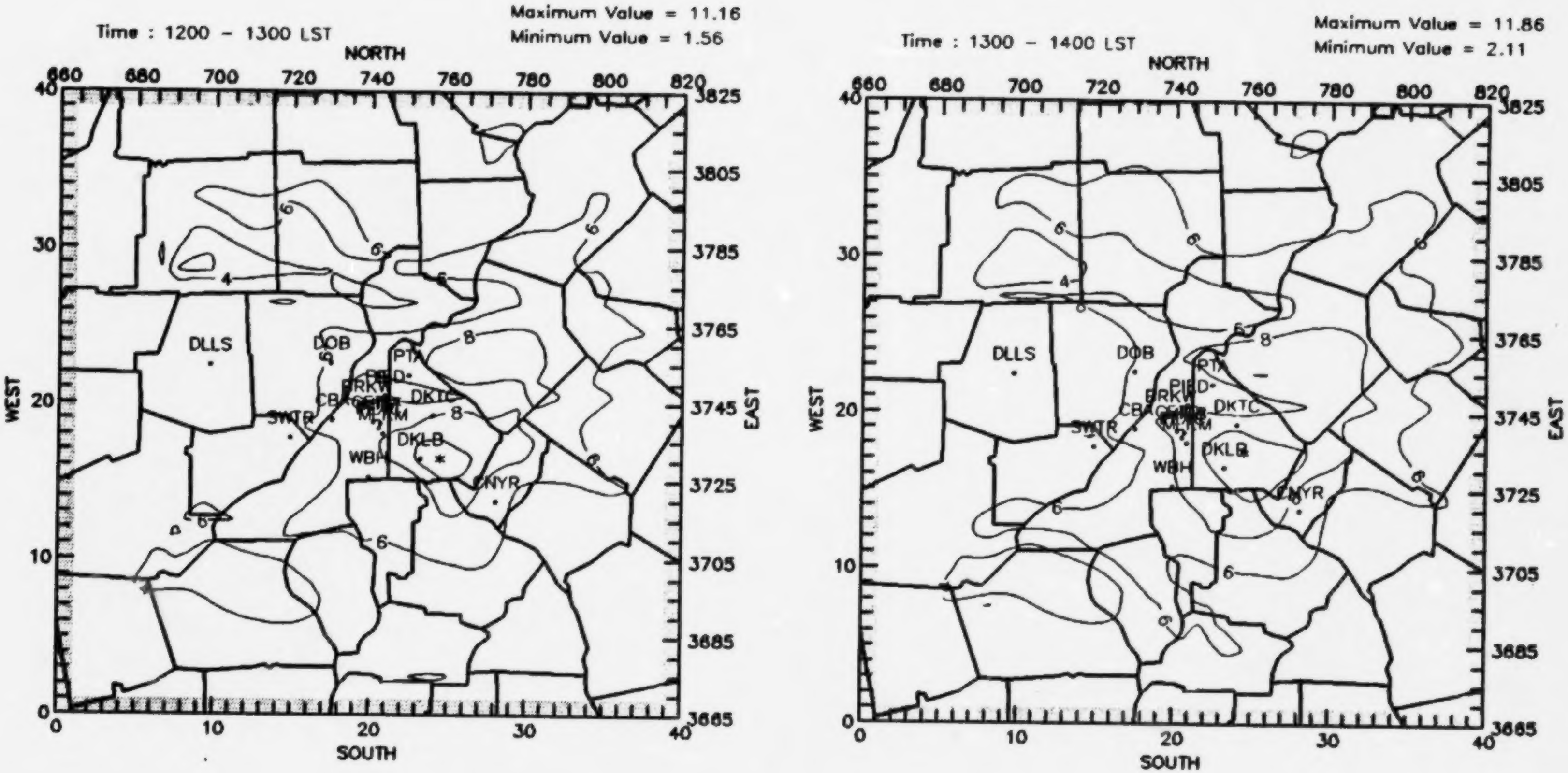
Maximum Value = 5.78
Minimum Value = 1.69

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIRD
BRKW
CBA
SWTR
DKTC
DKLB
WBH
CNYR
4

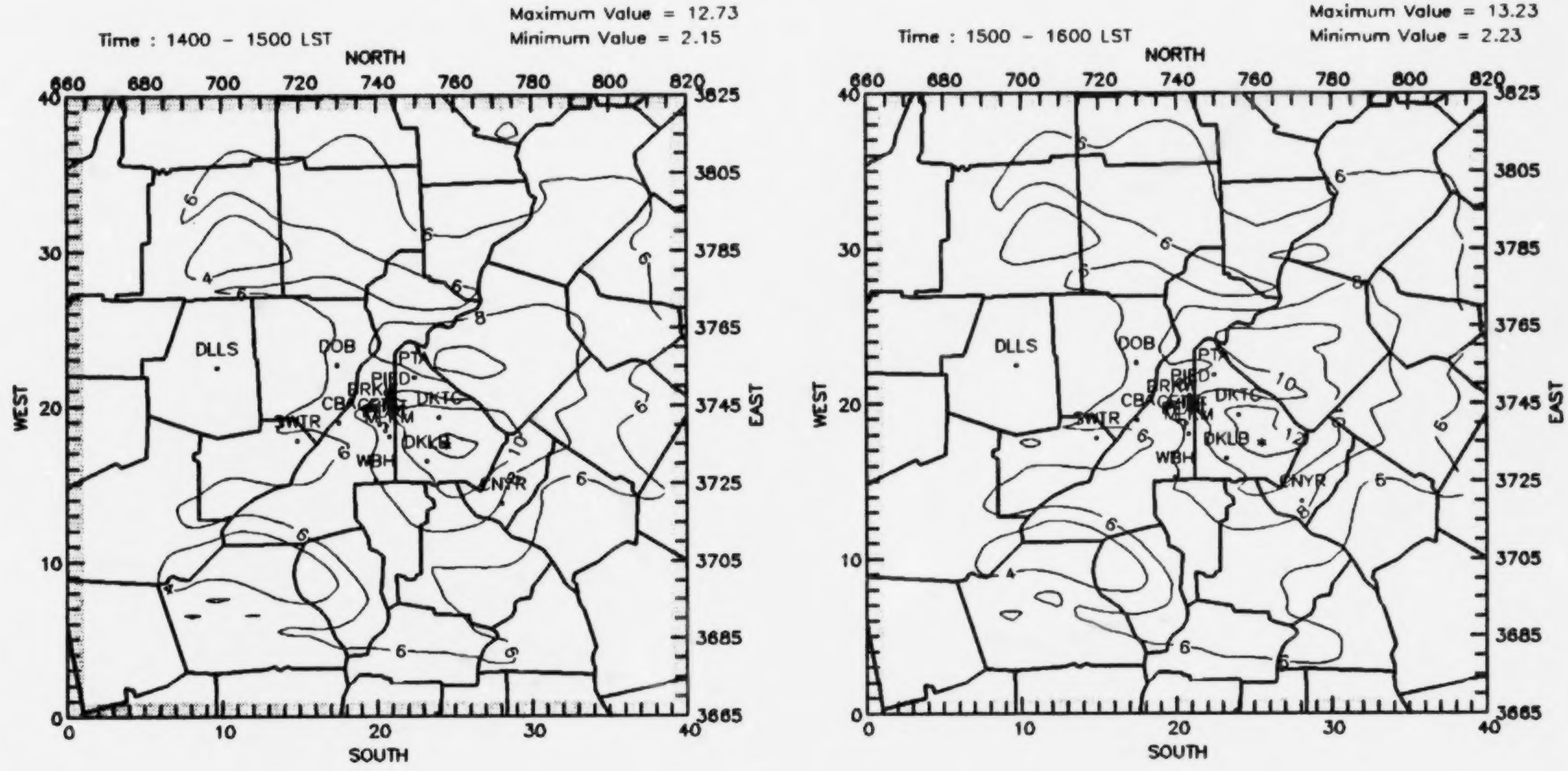
Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)


Time : 1000 - 1100 LST
Maximum Value = 7.84
Minimum Value = 1.58
Time : 1100 - 1200 LST
Maximum Value = 9.82
Minimum Value = 1.54
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIRD
BRKW
CBA
SWTR
BKTC
DKTC
DKLB
WBH
ENYR
4
6

Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)


Time : 1200 - 1300 LST
Maximum Value = 11.16
Minimum Value = 1.56
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTX
PIED
BRKW
CBA
SWTR
DKTC
MLTM
DKLB
WBH
CNYR
4
6
8
Time : 1300 - 1400 LST
Maximum Value = 11.86
Minimum Value = 2.11

Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)


Time : 1400 - 1500 LST

Maximum Value = 12.73

Minimum Value = 2.15

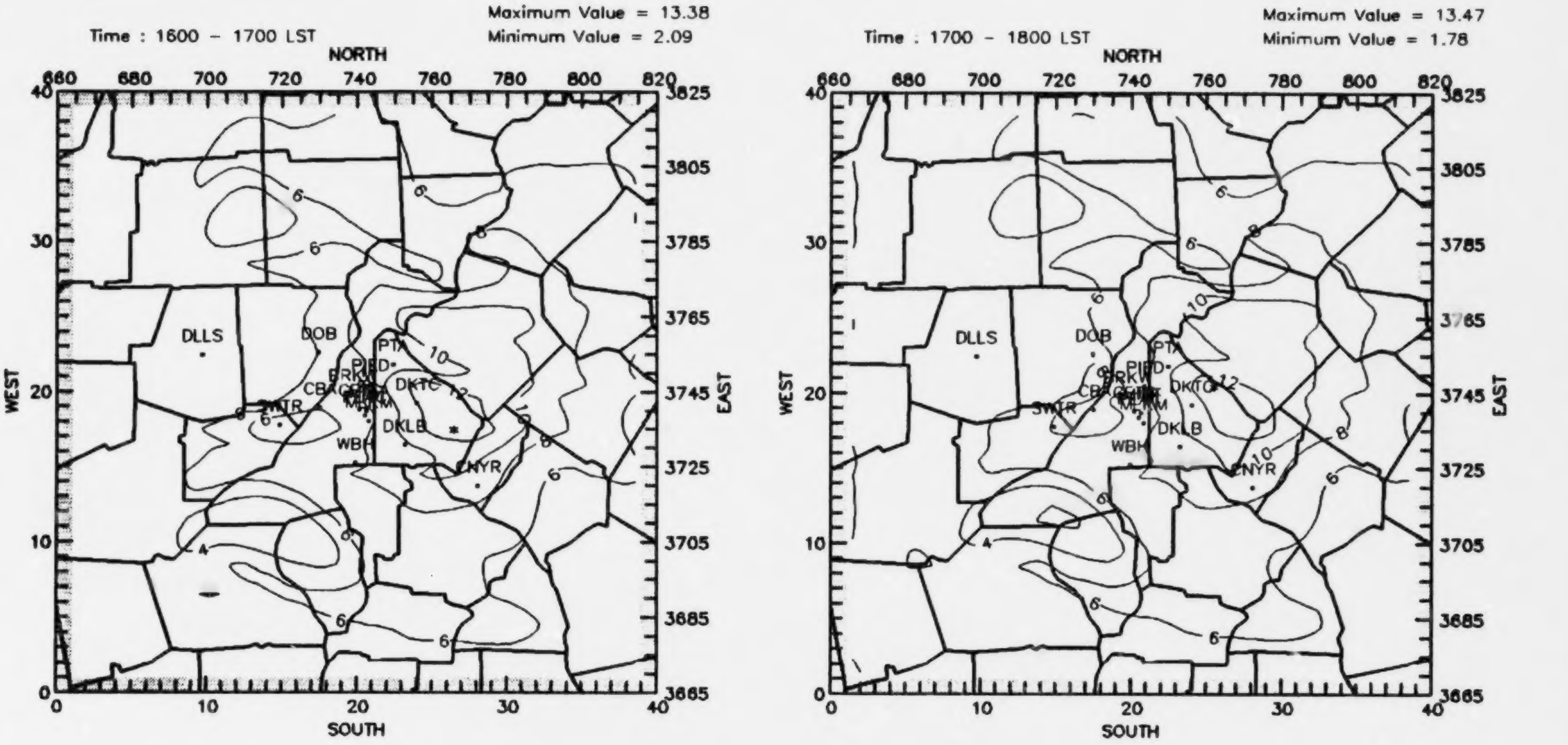
Time : 1500 - 1600 LST

Maximum Value = 13.23

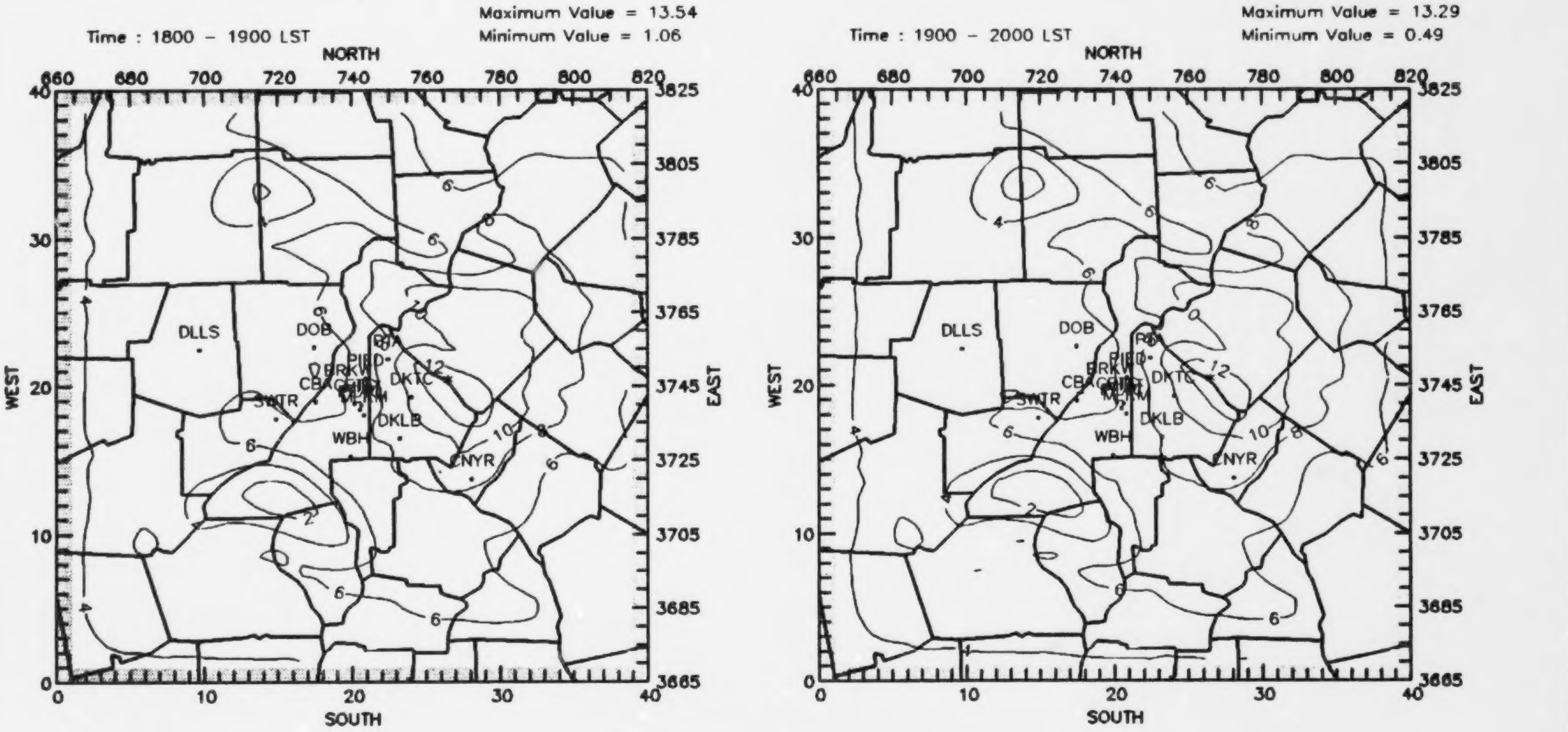
Minimum Value = 2.23

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIRD
BRKW
CBA
SWTR
DKTC
DKLB
WBH
CNYR
4
6
8
10
12

Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)


Time : 1600 - 1700 LST
Maximum Value = 13.38
Minimum Value = 2.09
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBAC
DKTC
SWTR
WBH
DKLB
CNYR
4
6
8
10
12
Time : 1700 - 1800 LST
Maximum Value = 13.47
Minimum Value = 1.78

Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)

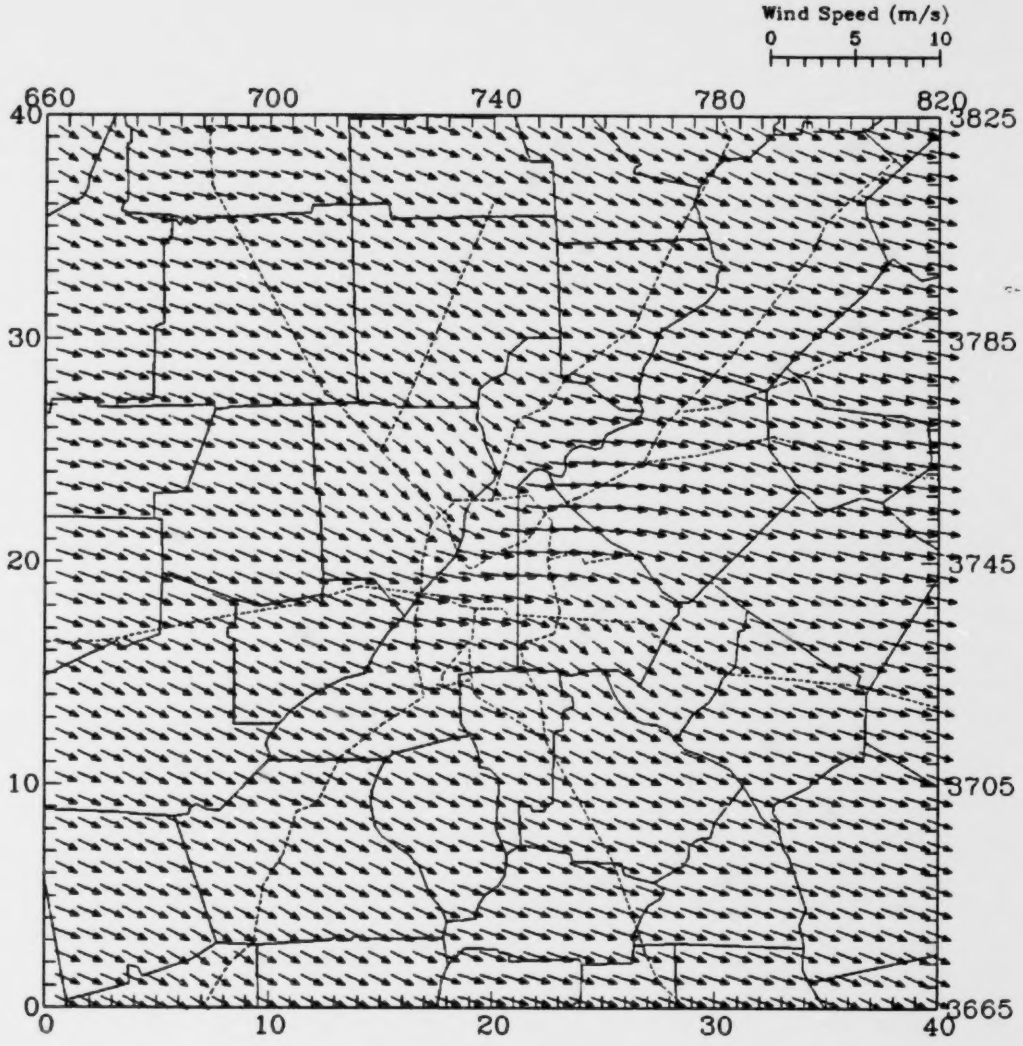


Time : 1800 - 1900 LST
Maximum Value = 13.54
Minimum Value = 1.06
Time : 1900 - 2000 LST
Maximum Value = 13.29
Minimum Value = 0.49
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PIRD
BRKW
CBA
DKTC
SWTR
WBH
DKLB
CNYR
2
4
6
8
10
12

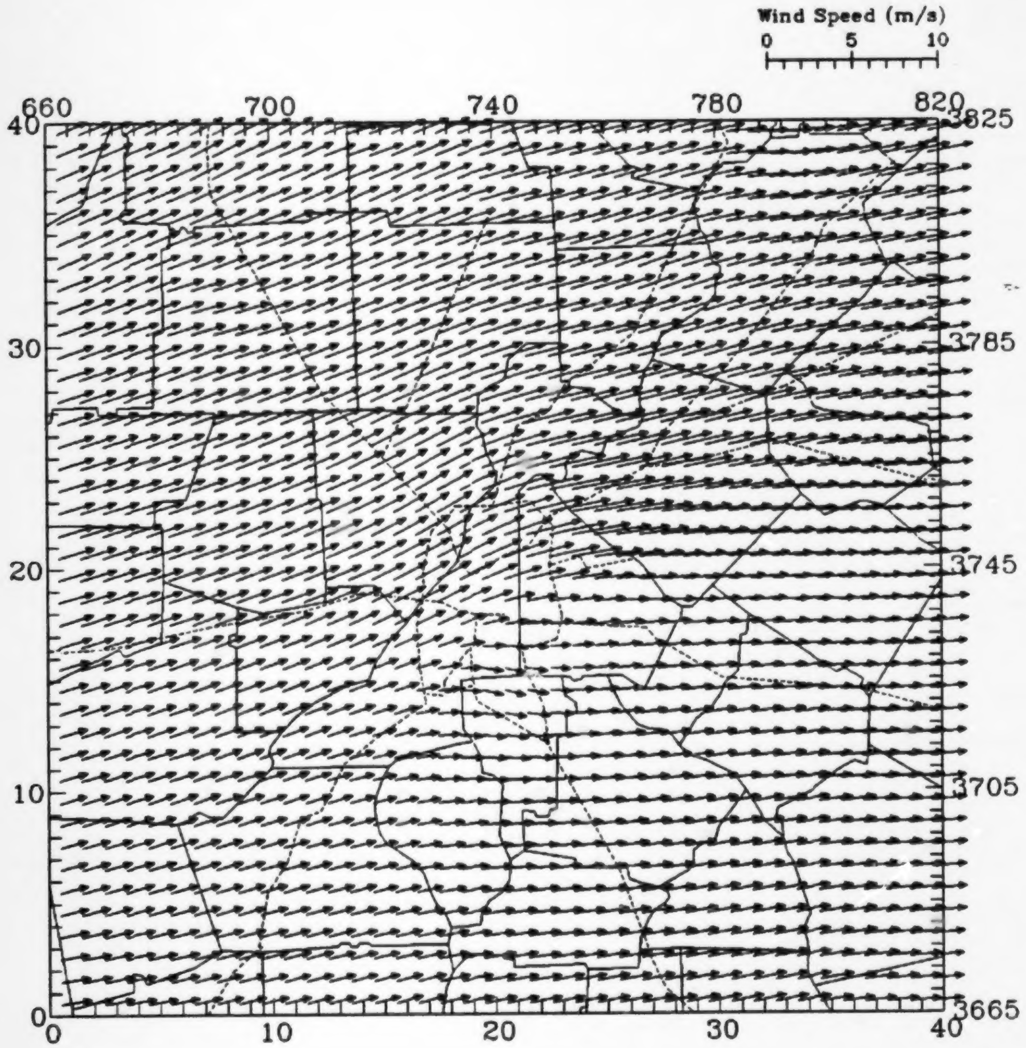
Ozone Concentration Evaluation run #1, June 4, 1984 (pphm)

Appendix D

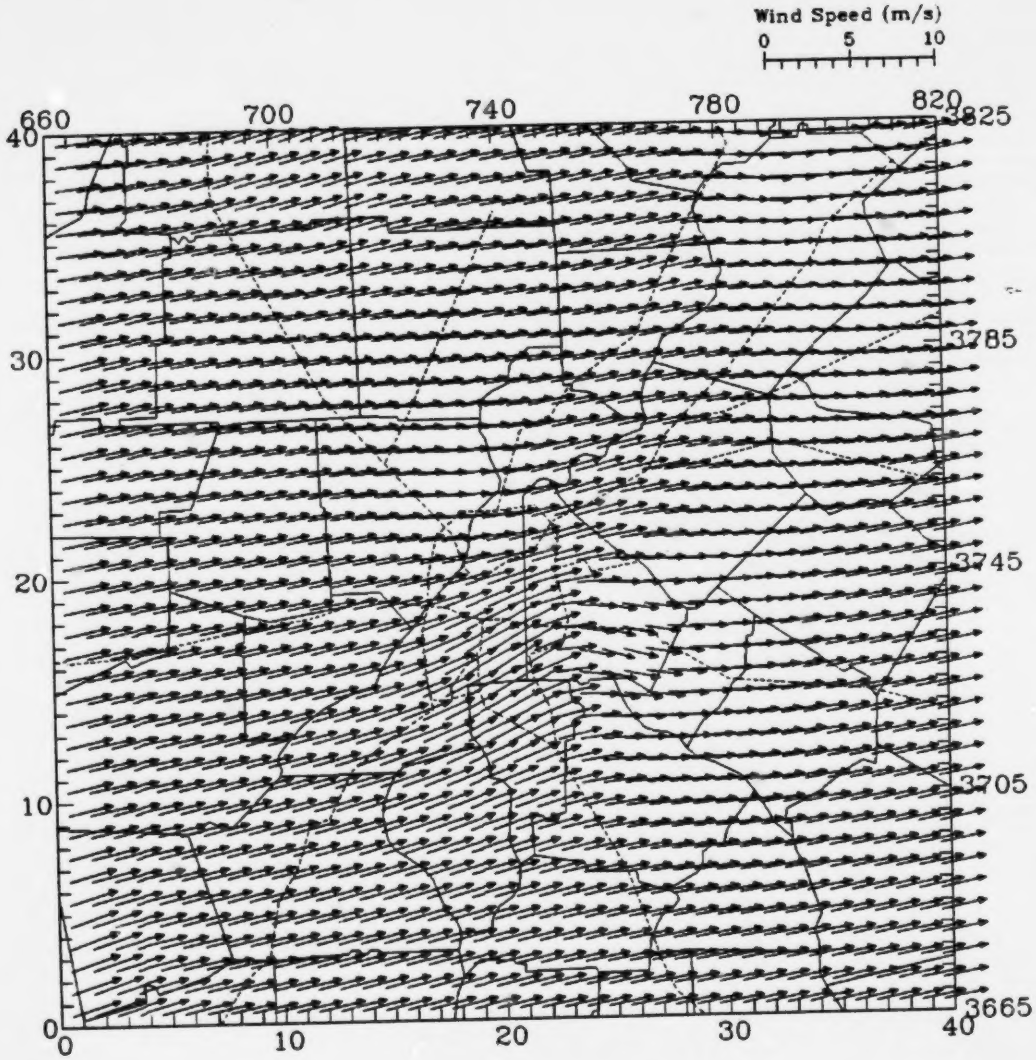
HOURLY WIND FIELDS FOR UAM LAYER 1 USED IN DIAGNOSTIC RUN 2 (BASE CASE SIMULATION WITH BIOGENICS)


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

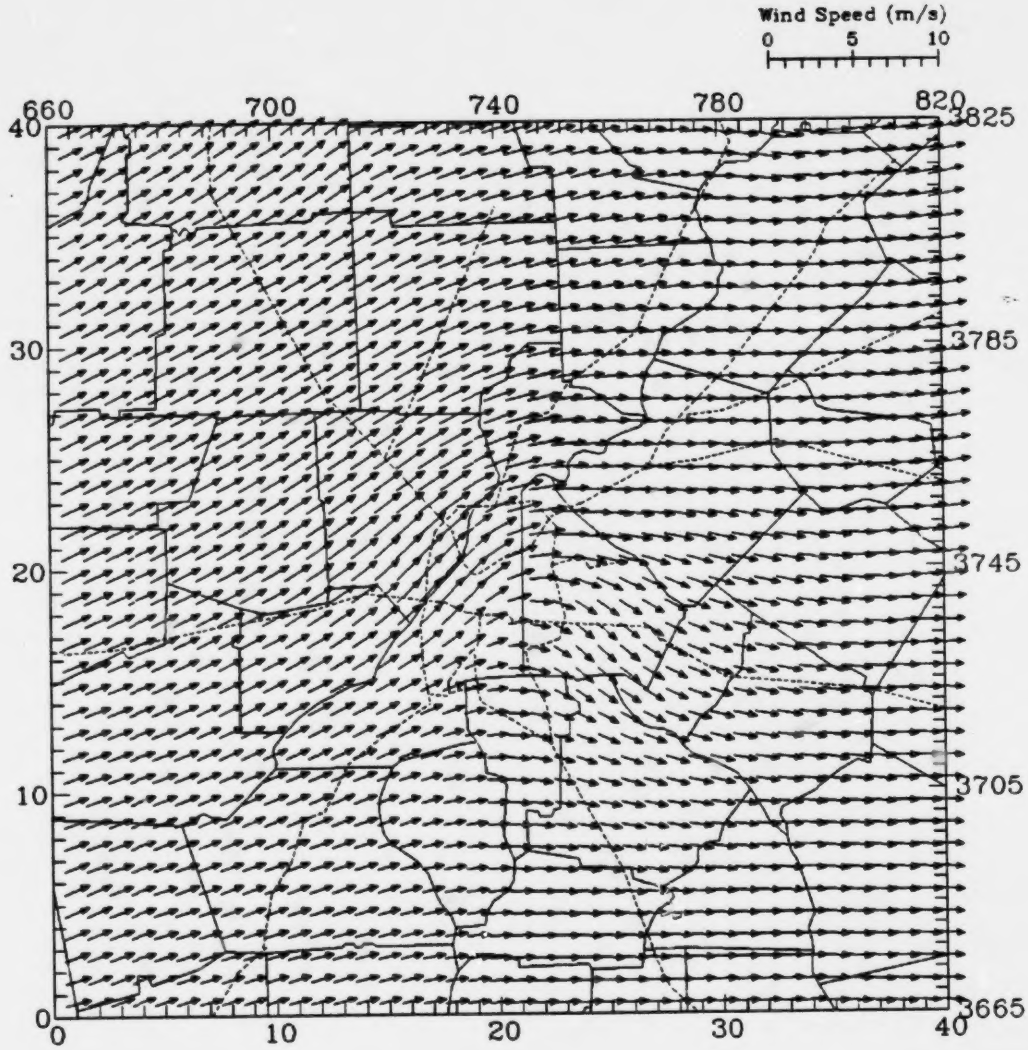
Atlanta PLANR Winds
Layer 1 at hour 10 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

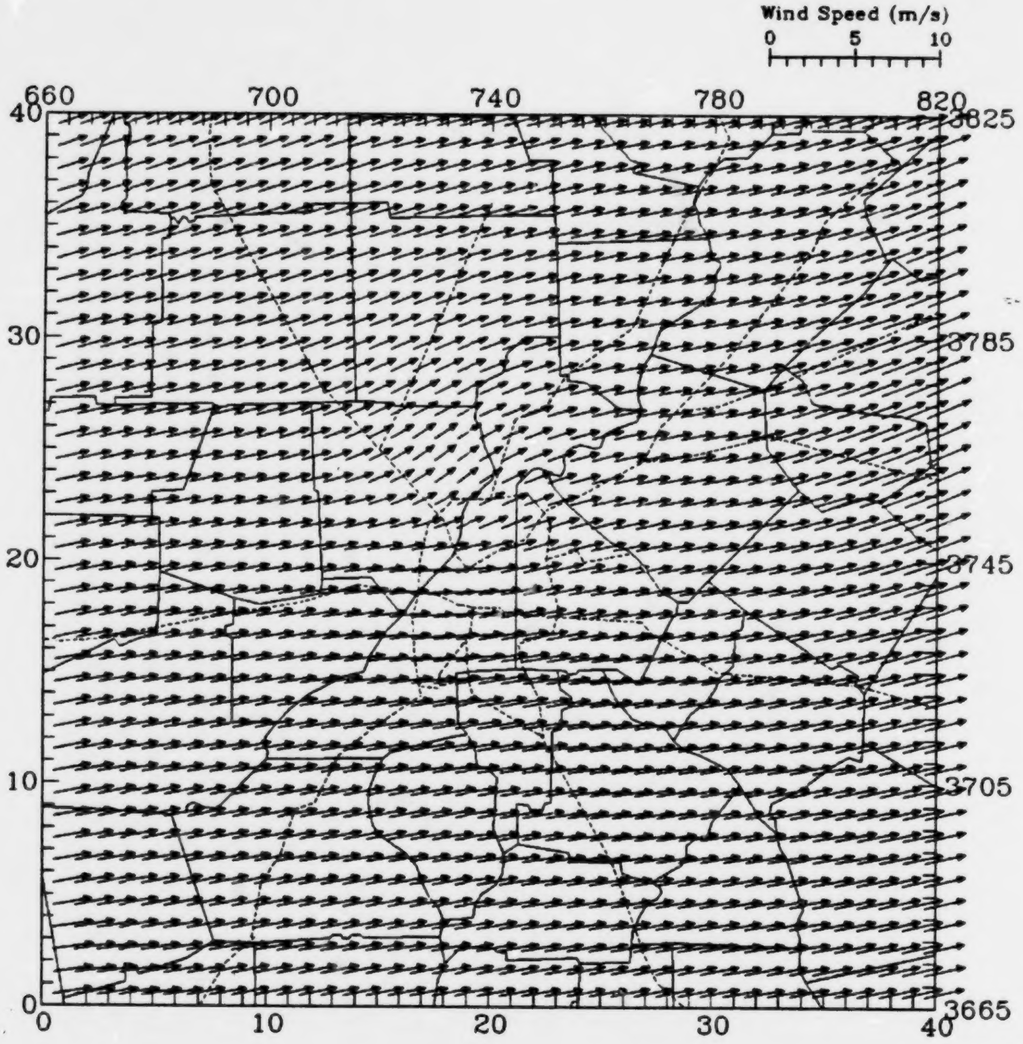
Atlanta PLANR Winds
Layer 1 at hour 11 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

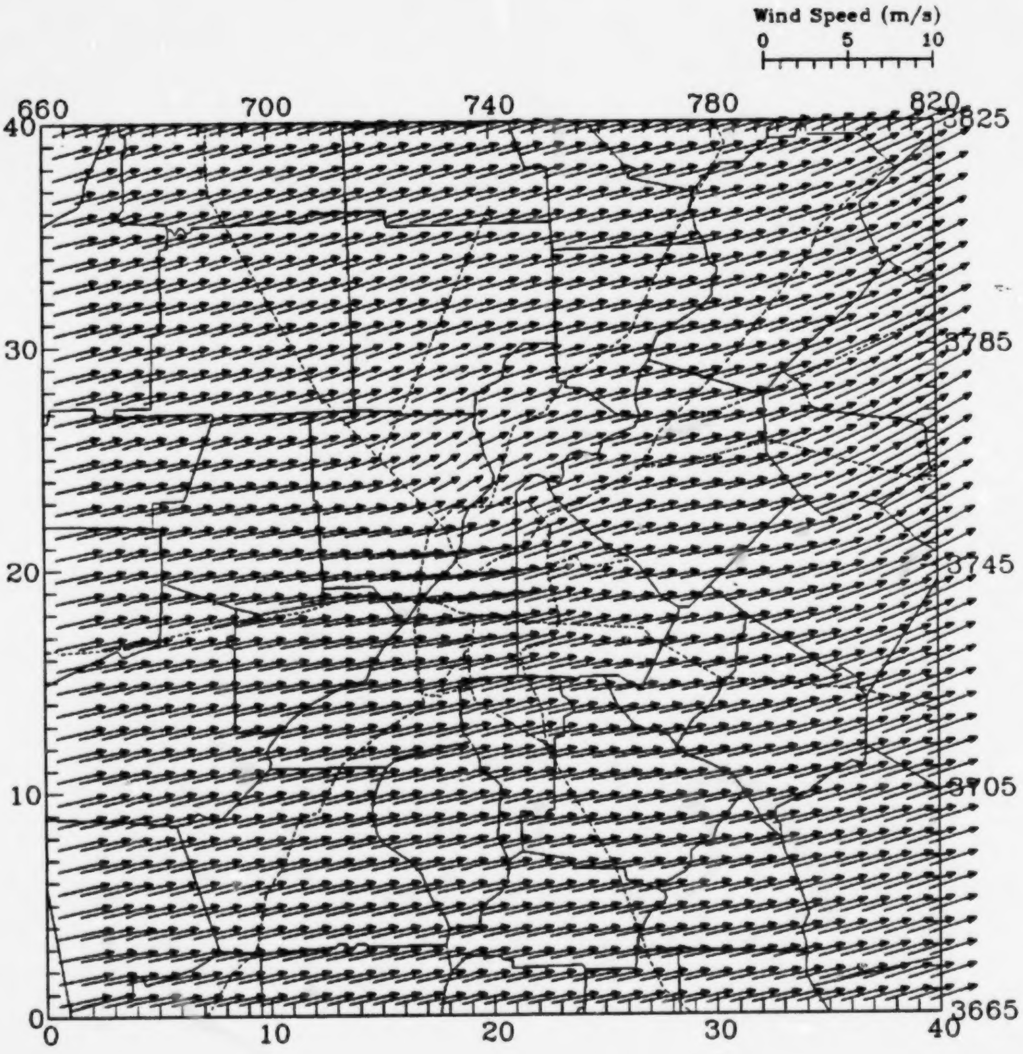
Atlanta PLANR Winds
Layer 1 at hour 12 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

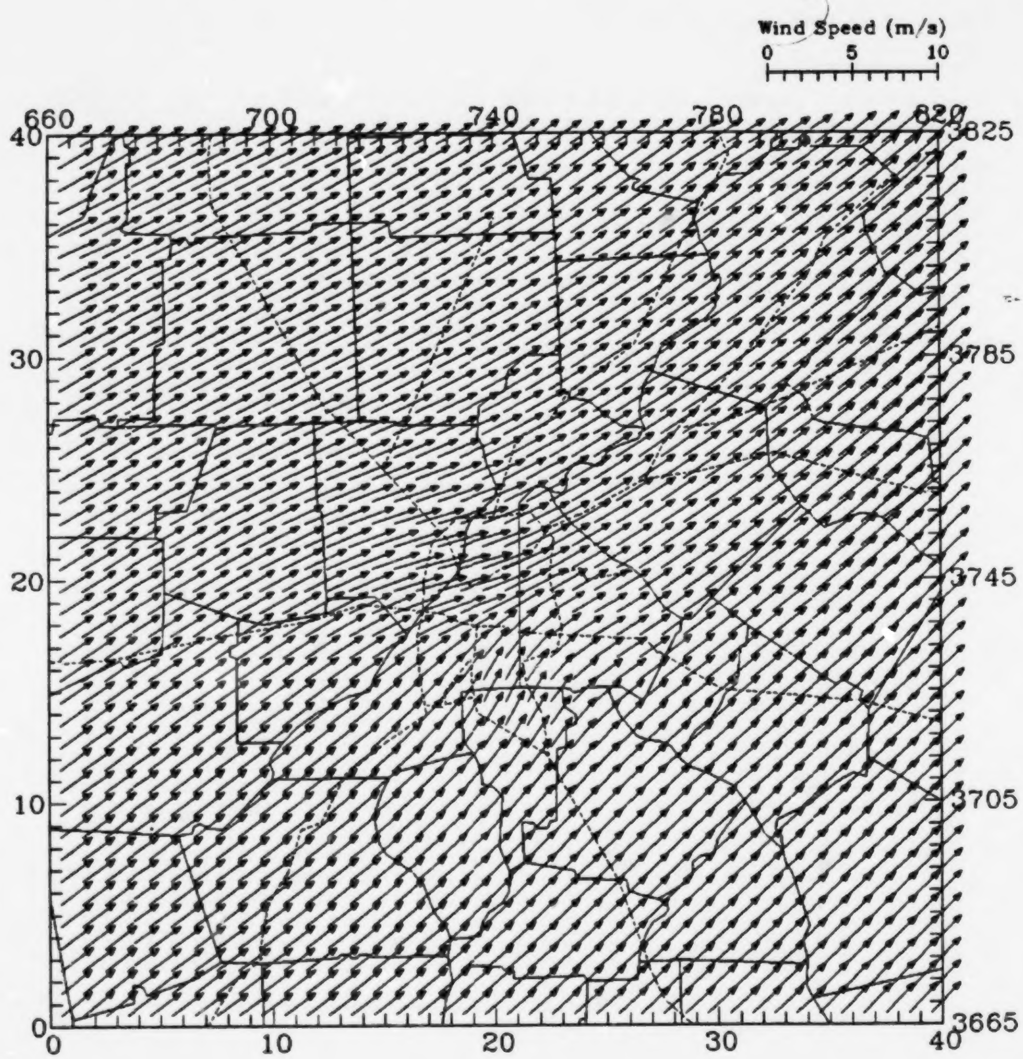
Atlanta PLANR Winds
Layer 1 at hour 13 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

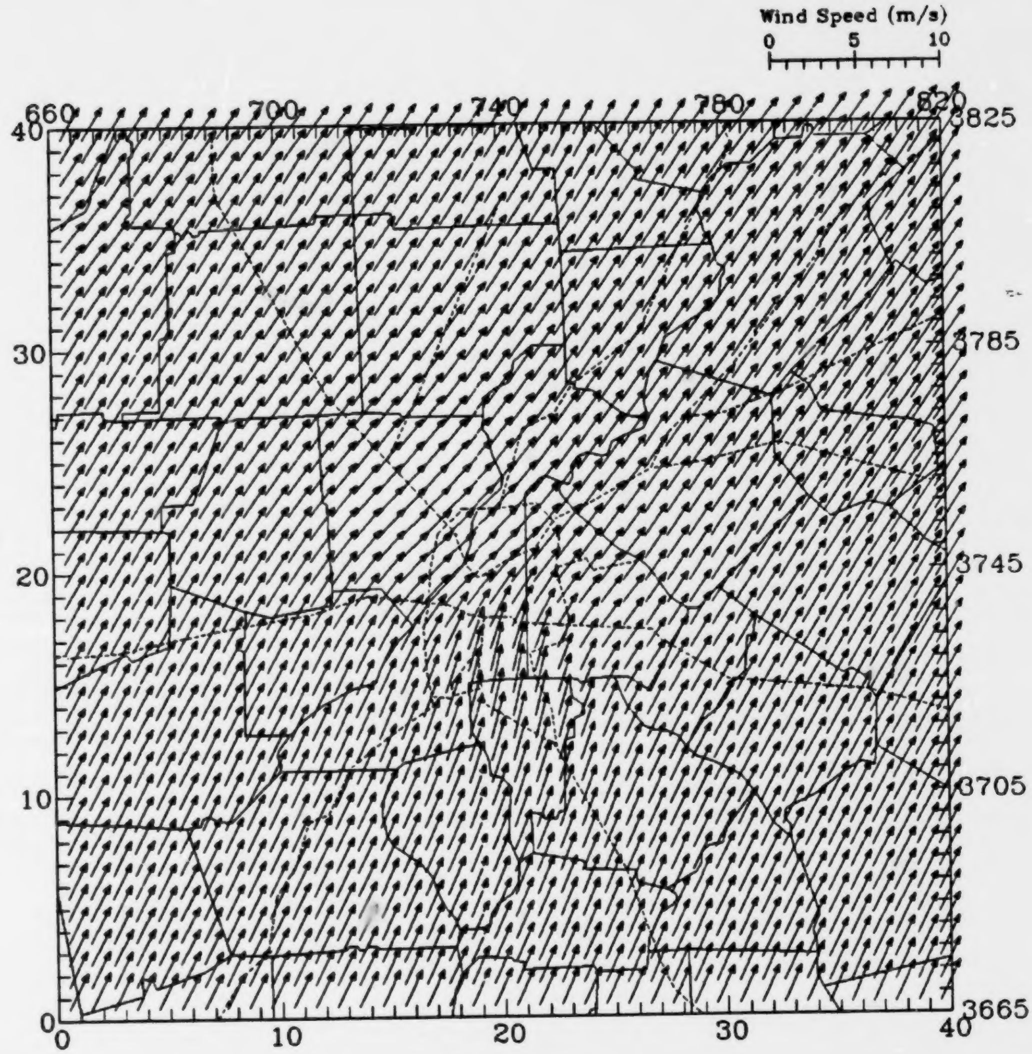
Atlanta PLANR Winds
Layer 1 at hour 14 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

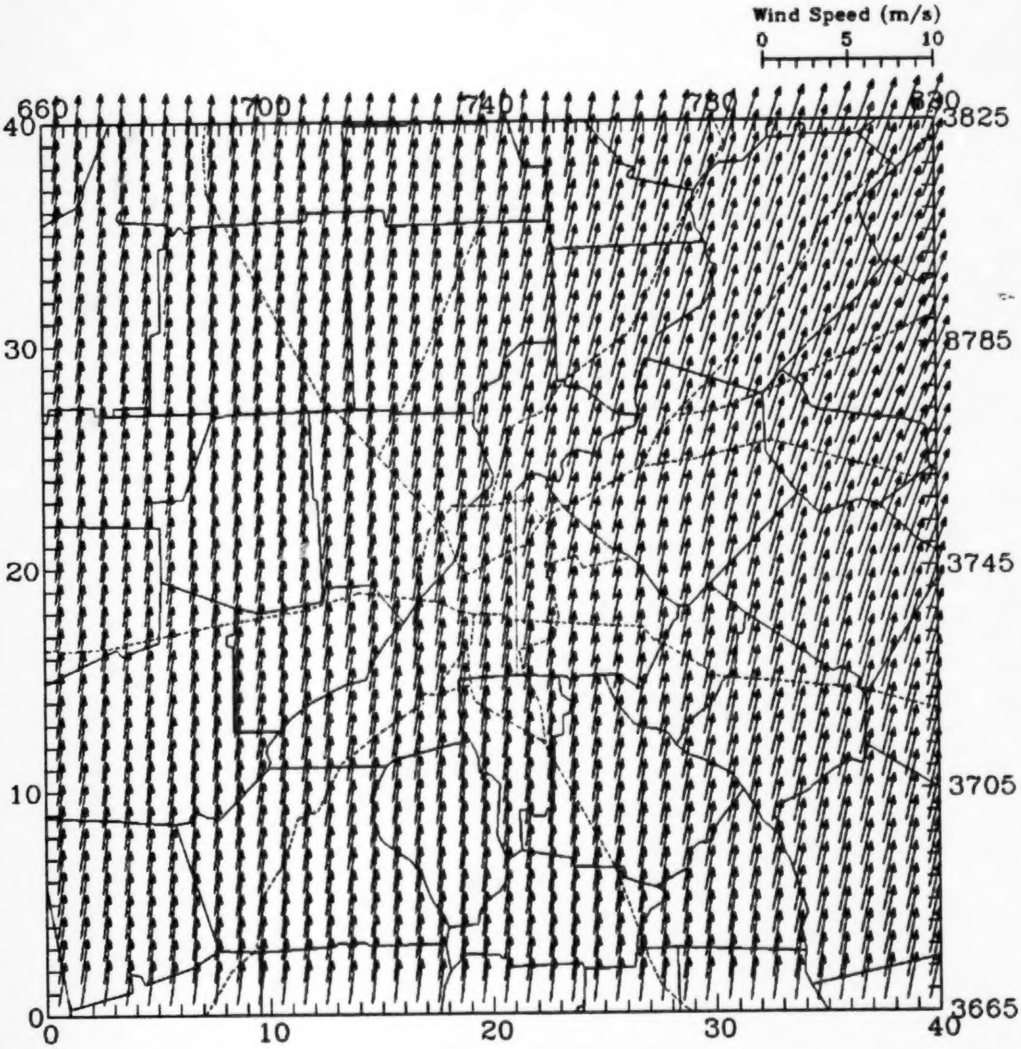
Atlanta PLANR Winds
Layer 1 at hour 15 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

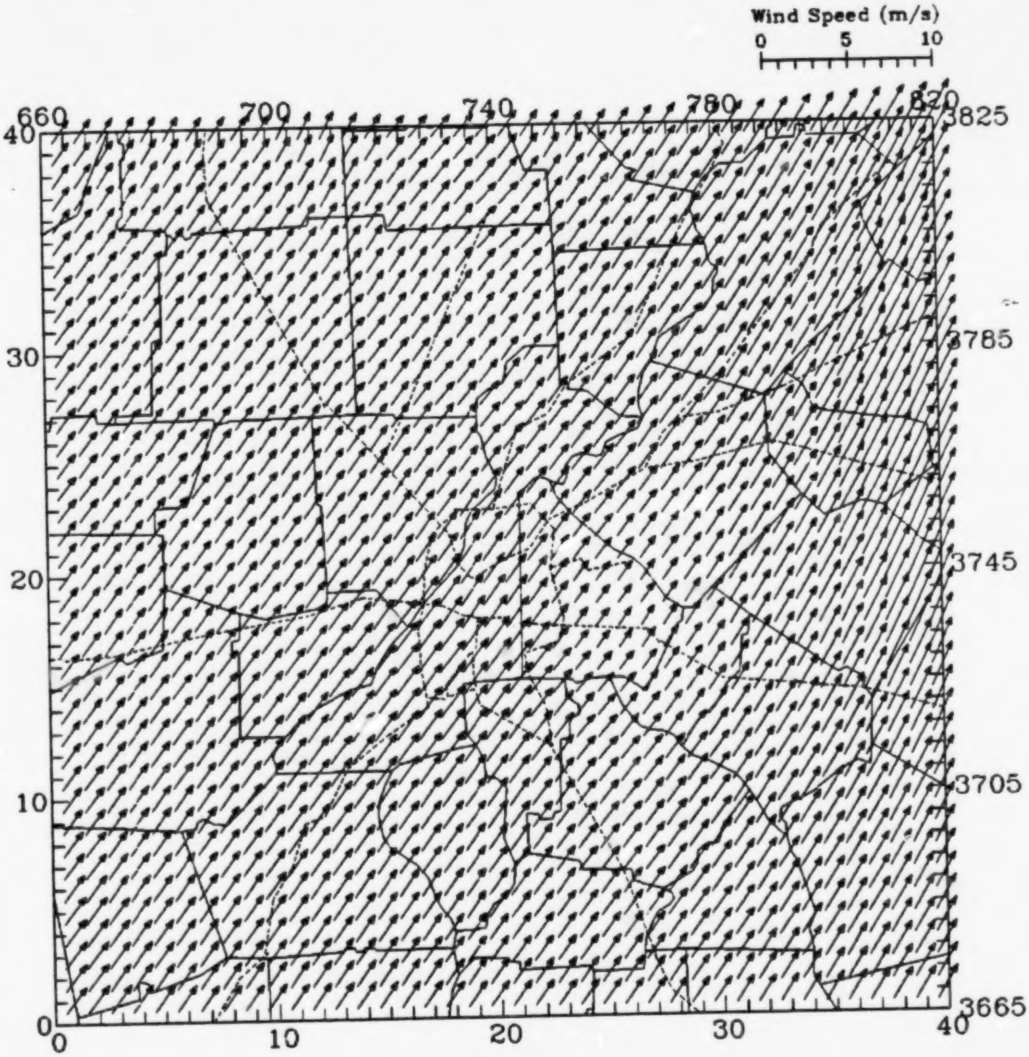
Atlanta PLANR Winds
Layer 1 at hour 16 on 84156


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

Atlanta PLANR Winds
Layer 1 at hour 17 on 84156

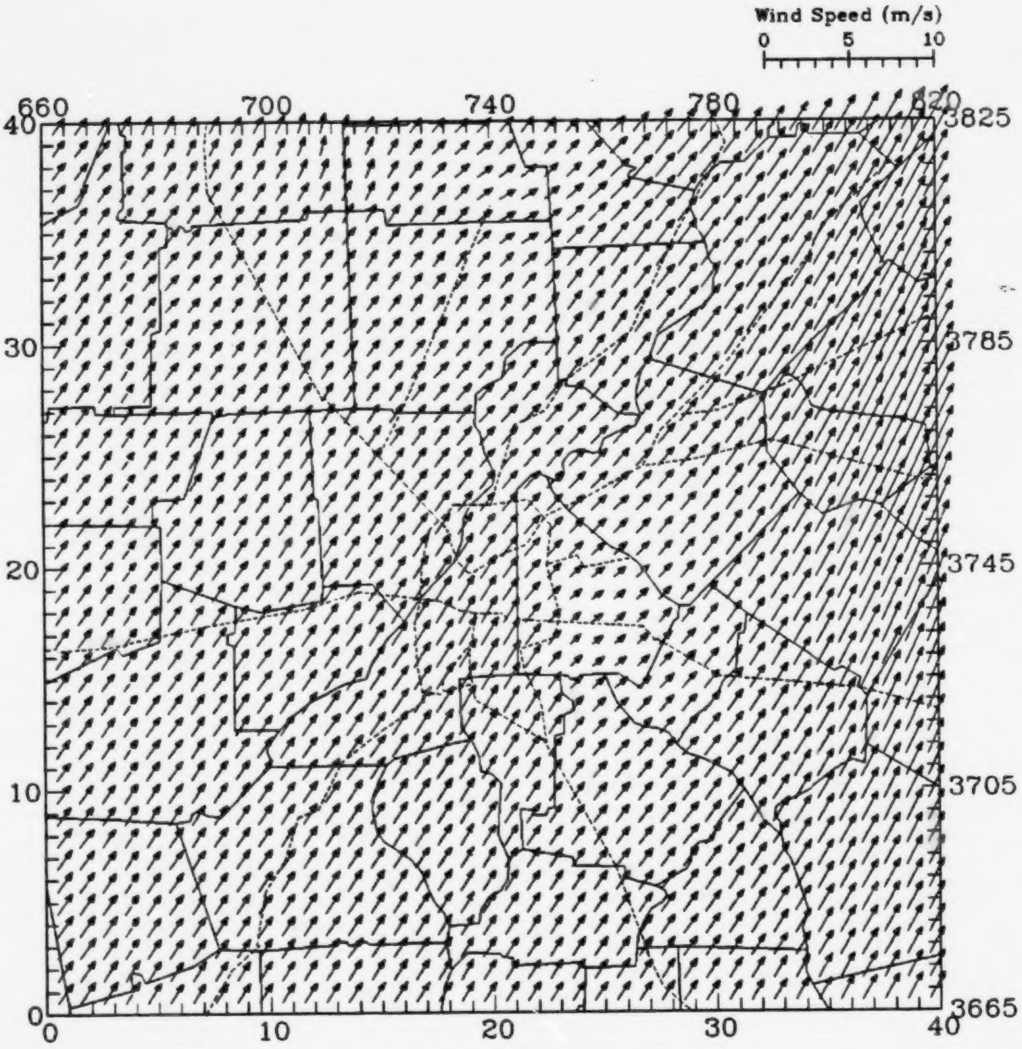

Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

Atlanta PLANR Winds
Layer 1 at hour 18 on 84156



Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

Atlanta PLANR Winds
Layer 1 at hour 19 on 84156

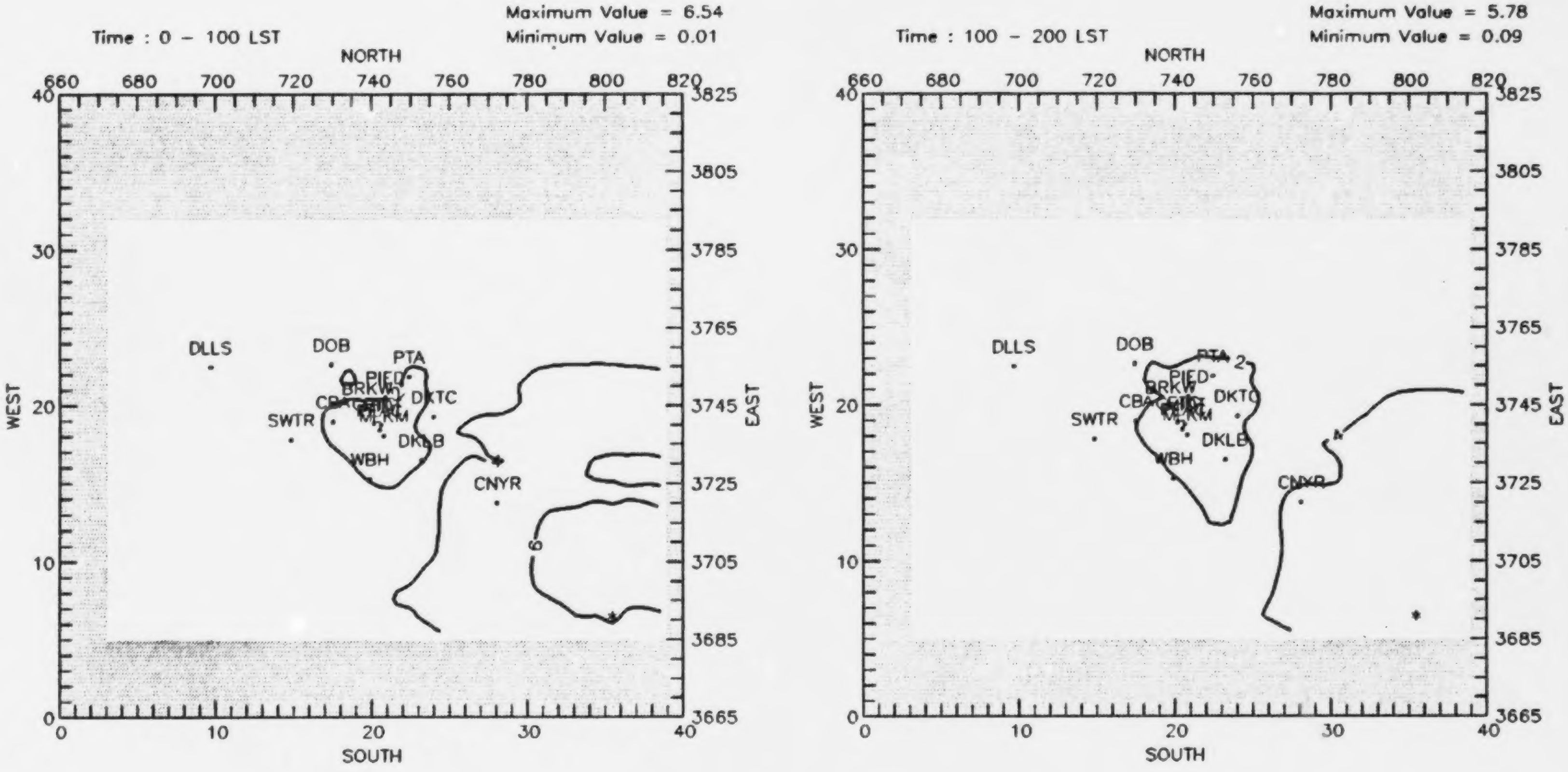


Wind Speed (m/s)
0
5
10
660
700
740
780
820
3825
3785
3745
3705
3665
40
30
20
10
0
0
10
20
30
40

Atlanta PLANR Winds
Layer 1 at hour 20 on 84156

Appendix E

HOURLY PREDICTED OZONE CONCENTRATIONS (pphm) FOR DIAGNOSTIC RUN 2 (BASE CASE WITH BIOGENIC EMISSIONS)


Time : 0 - 100 LST

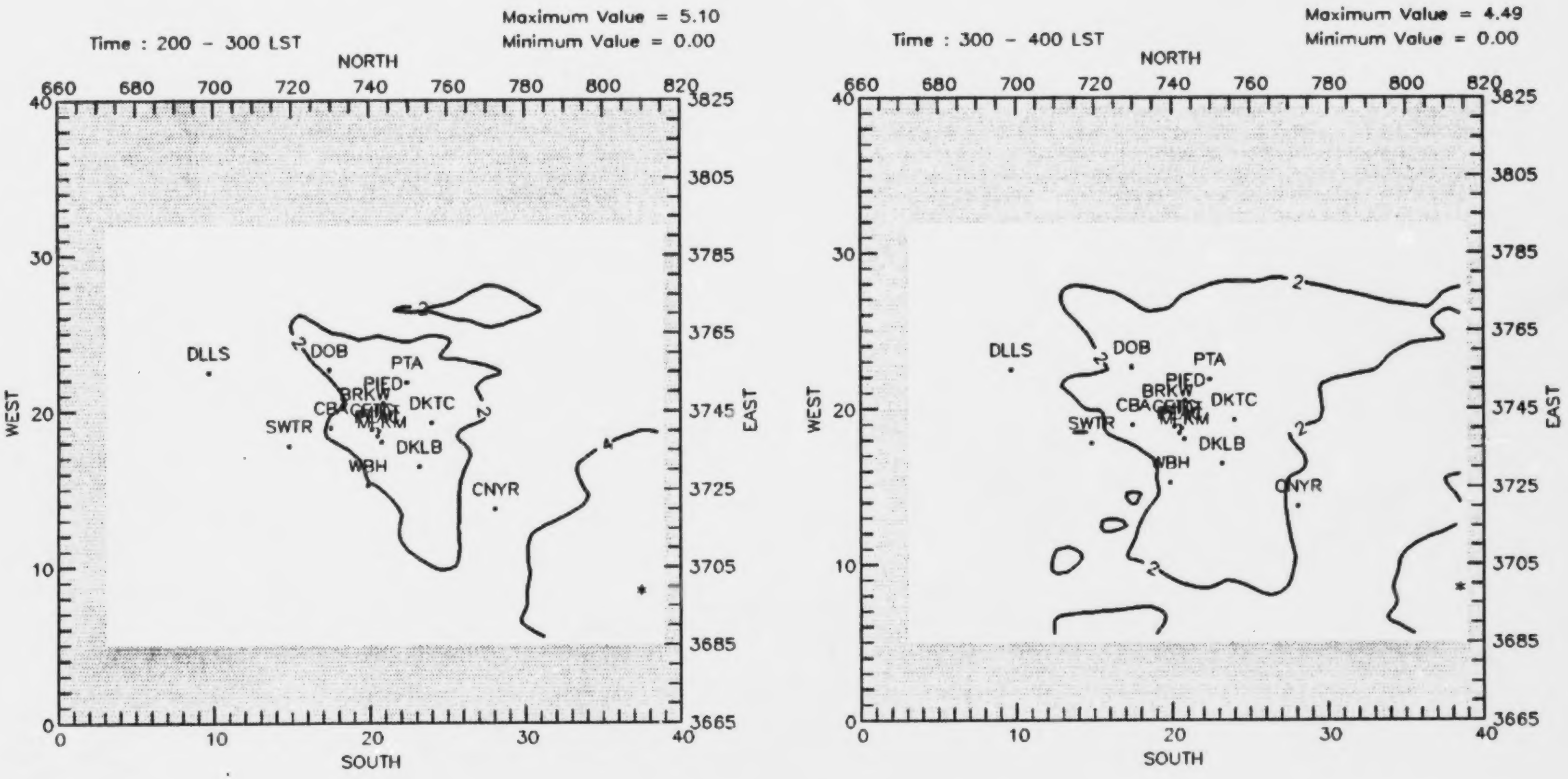
Maximum Value = 6.54
Minimum Value = 0.01

Time : 100 - 200 LST

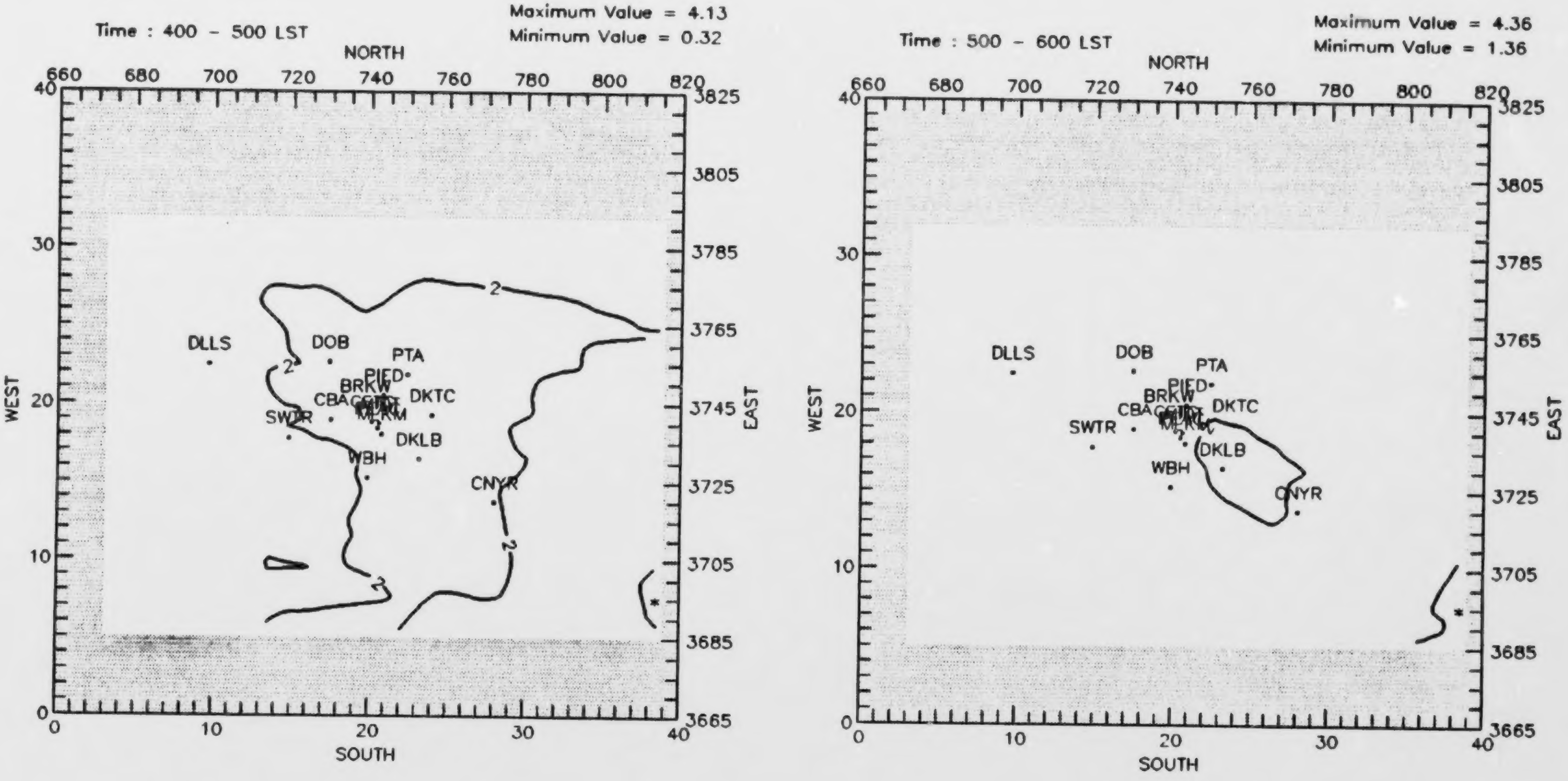
Maximum Value = 5.78
Minimum Value = 0.09

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
6
2
4

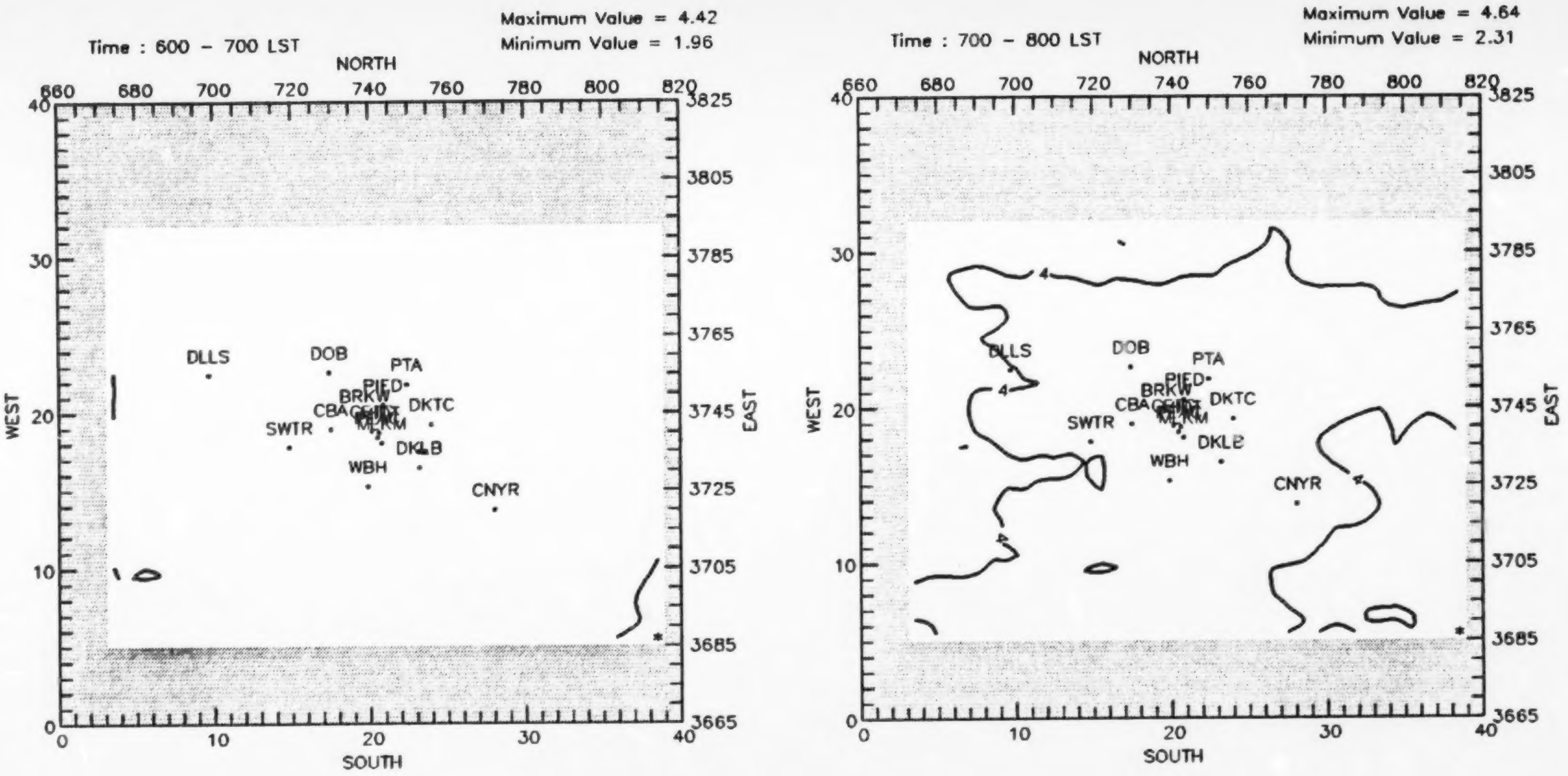
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)


Time : 200 - 300 LST
Maximum Value = 5.10
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
40
30
20
10
0
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
2
4
Time : 300 - 400 LST
Maximum Value = 4.49
Minimum Value = 0.00

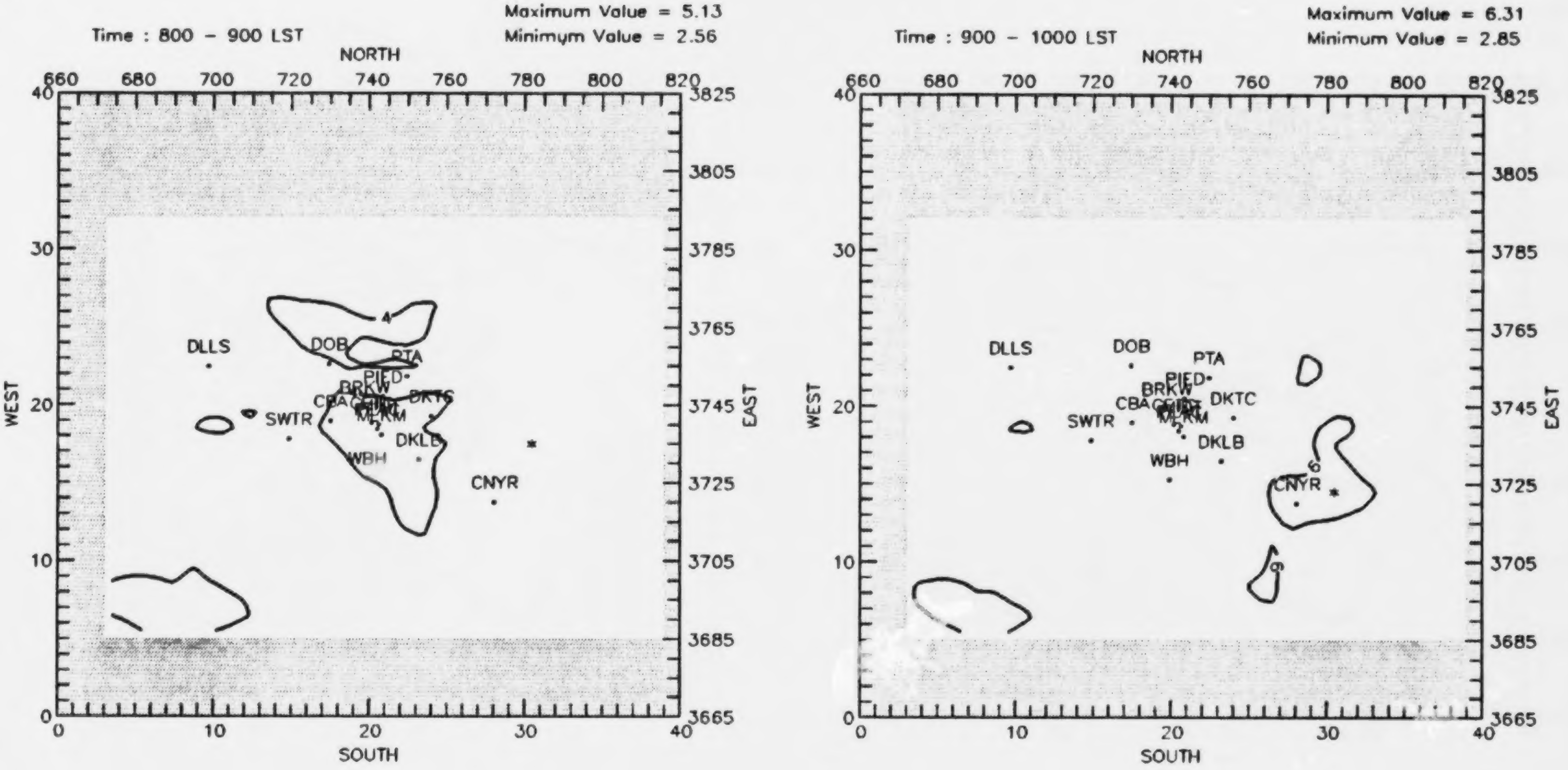
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)


Time : 400 - 500 LST
Maximum Value = 4.13
Minimum Value = 0.32
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
2
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
*
Time : 500 - 600 LST
Maximum Value = 4.36
Minimum Value = 1.36

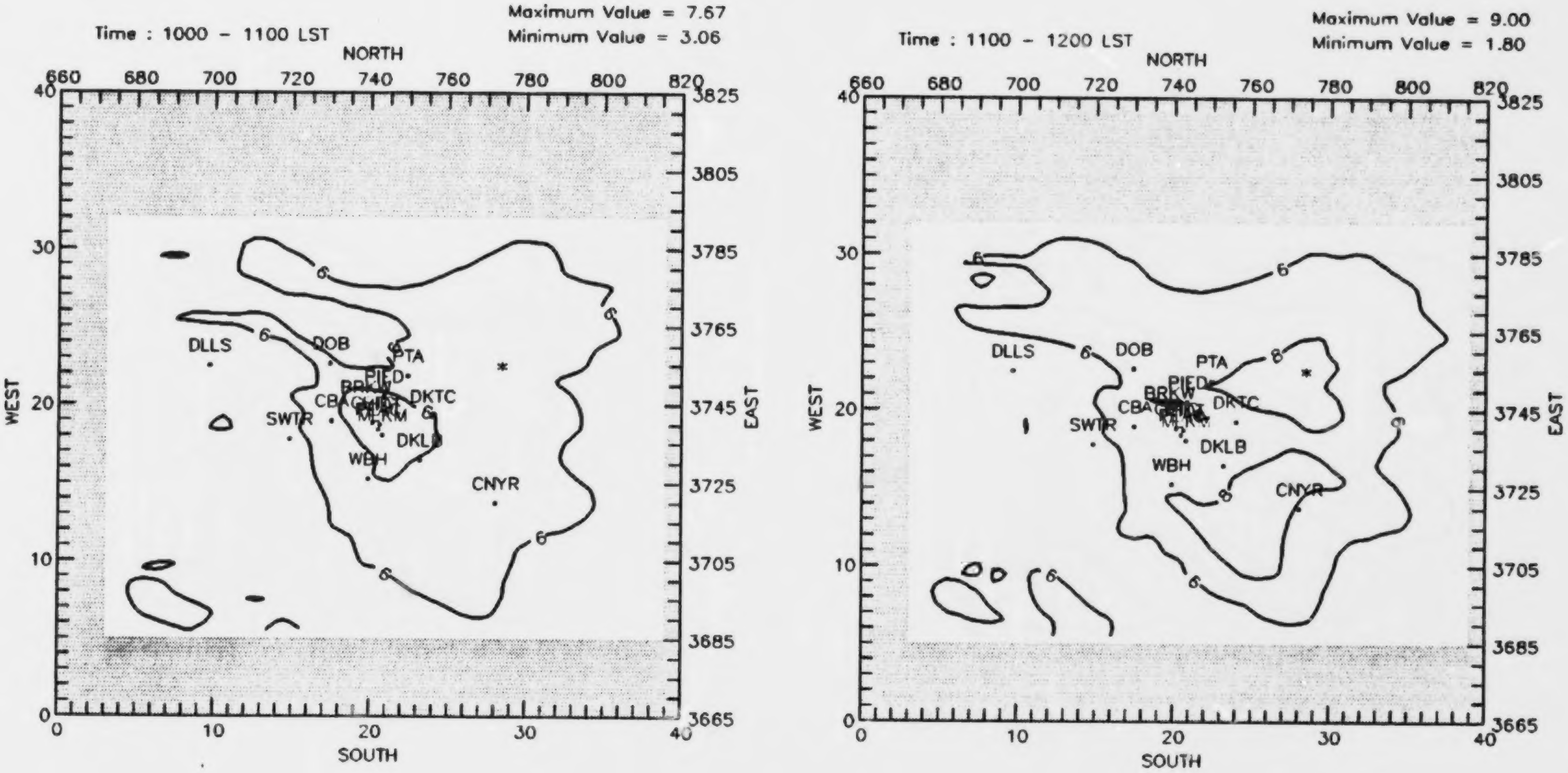
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)


Time : 600 - 700 LST
Maximum Value = 4.42
Minimum Value = 1.96
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
Time : 700 - 800 LST
Maximum Value = 4.64
Minimum Value = 2.31
4

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

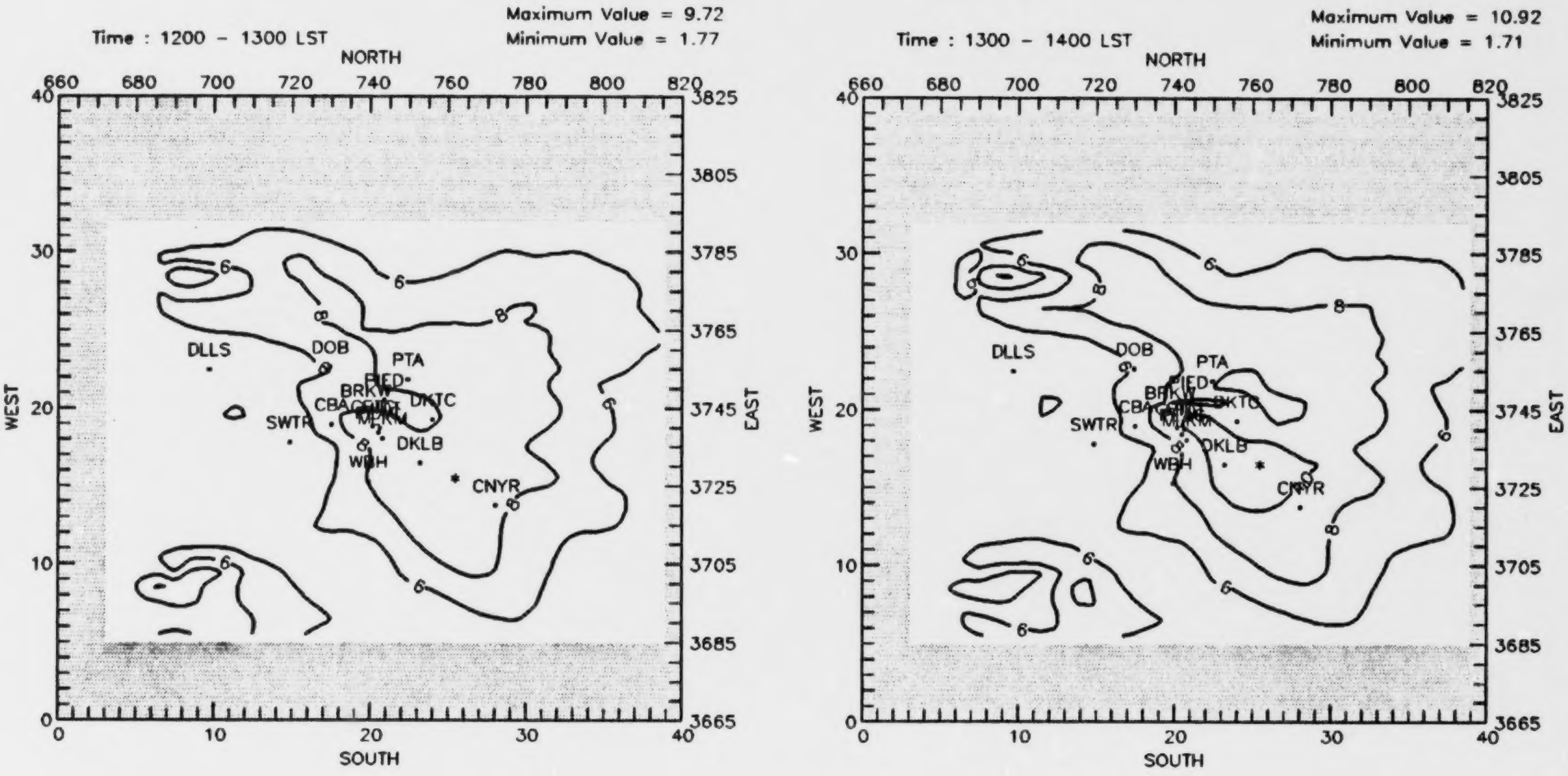

Time : 800 - 900 LST
Maximum Value = 5.13
Minimym Value = 2.56
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MRM
DKLB
WBH
CNYR
4
Time : 900 - 1000 LST
Maximum Value = 6.31
Minimum Value = 2.85
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MRM
DKLB
WBH
CNYR
6
6

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)



Time : 1000 - 1100 LST
Maximum Value = 7.67
Minimum Value = 3.06
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
6
Time : 1100 - 1200 LST
Maximum Value = 9.00
Minimum Value = 1.80
8

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)



Time : 1200 - 1300 LST

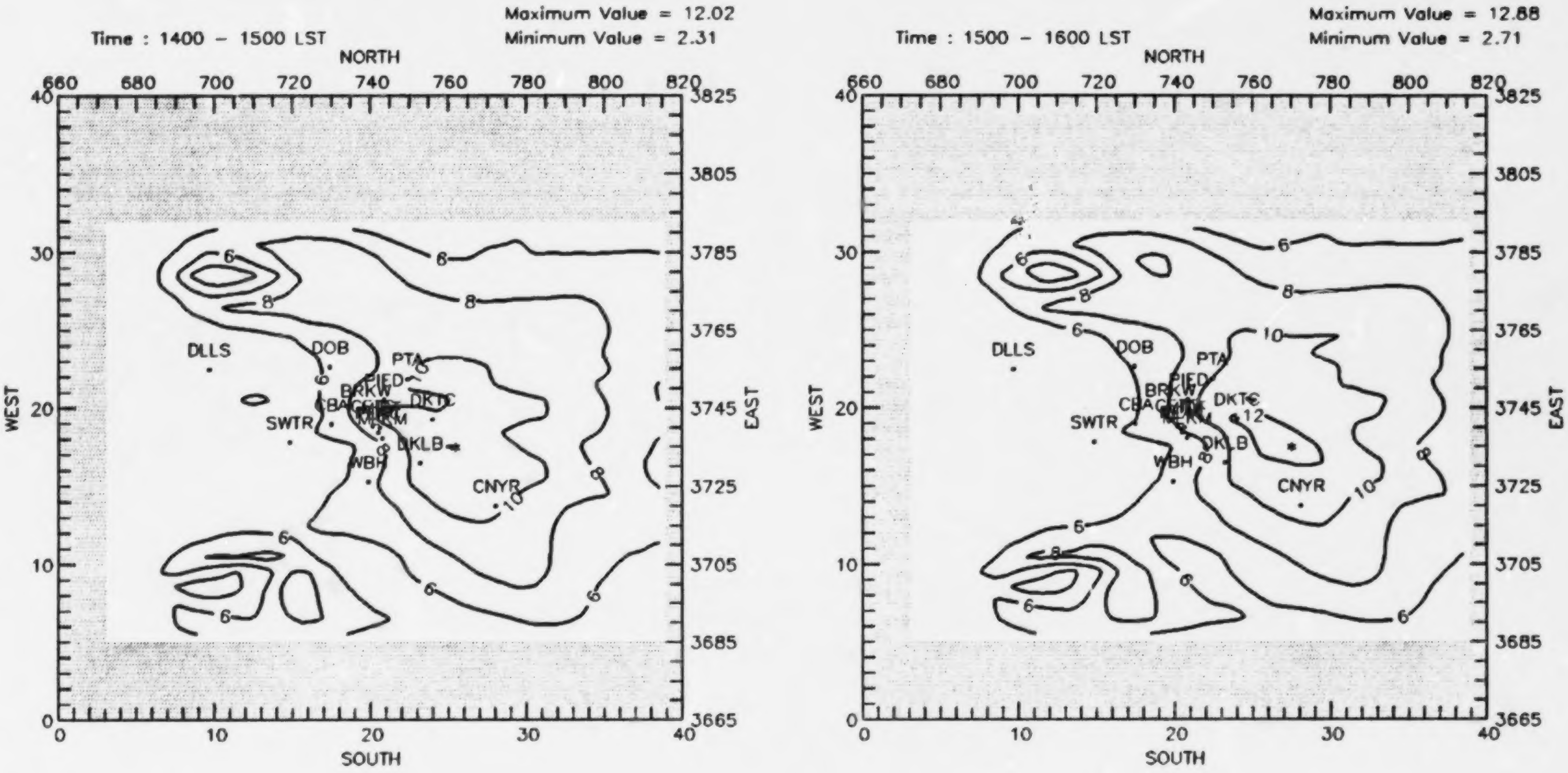
Maximum Value = 9.72
Minimum Value = 1.77

Time : 1300 - 1400 LST

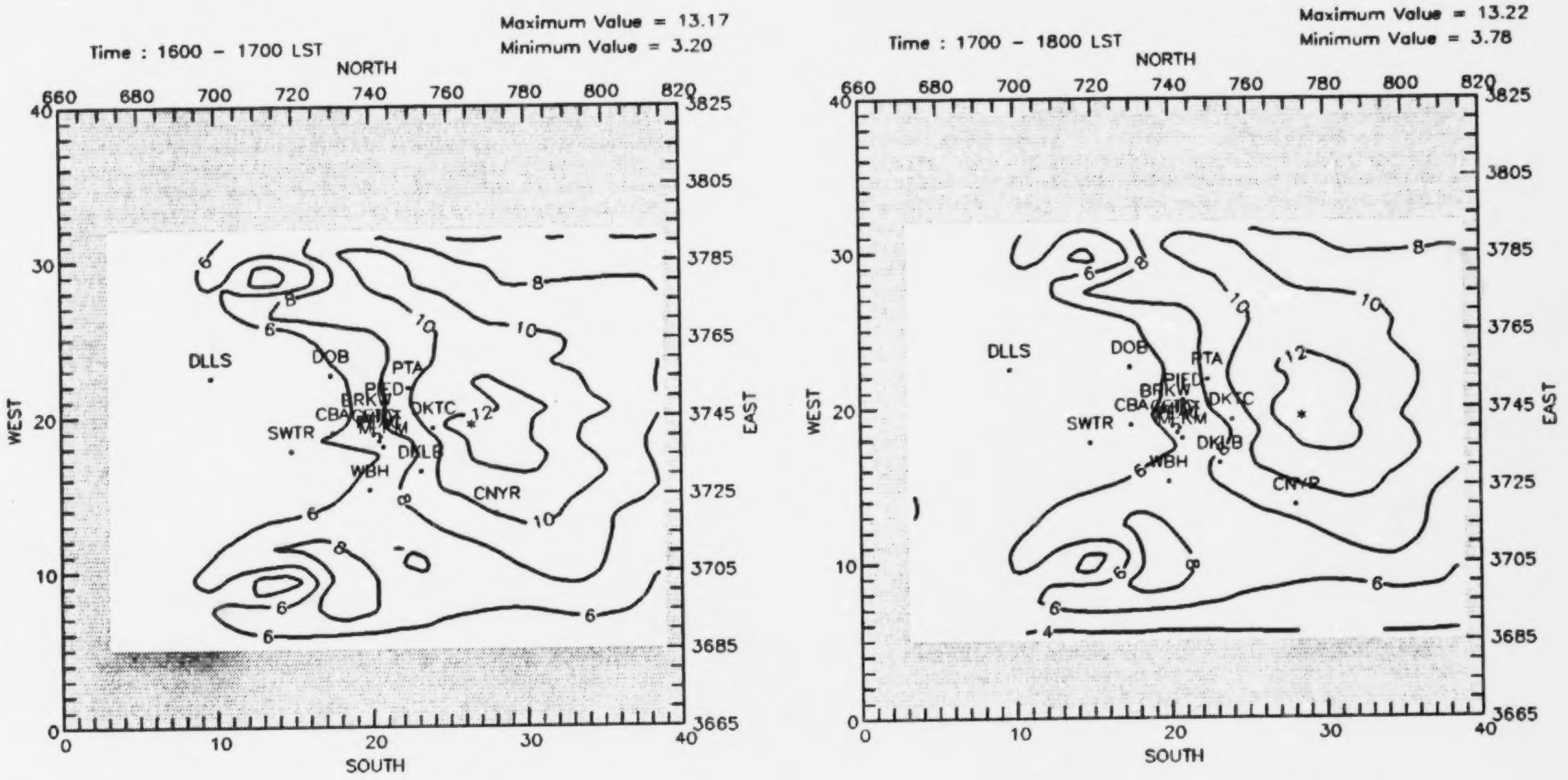
Maximum Value = 10.92
Minimum Value = 1.71

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
FIED
BRKW
CBA
DKTC
SWTR
WBH
DKLB
CNYR
6
8

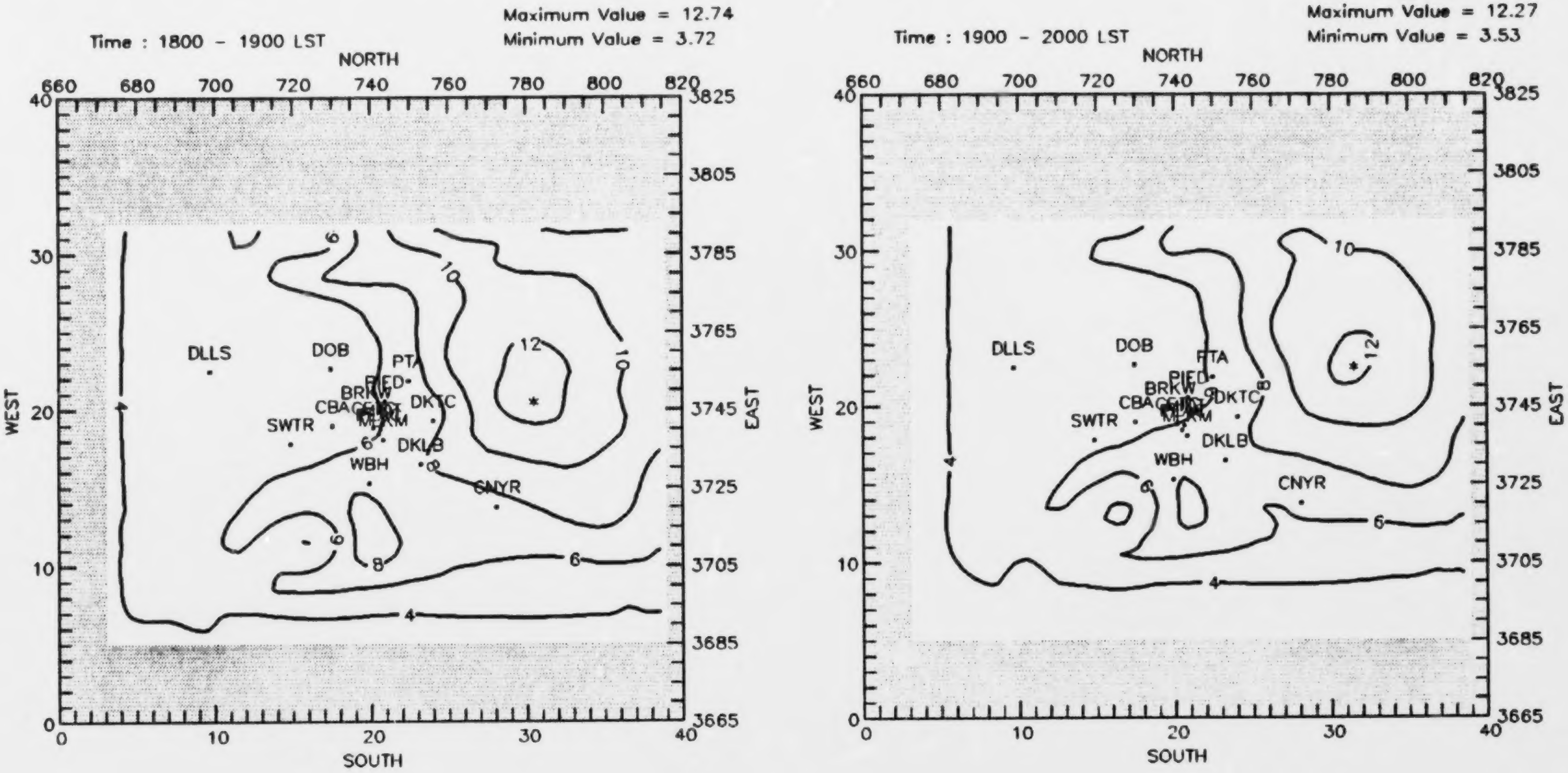
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)



Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)


Time : 1600 - 1700 LST
Maximum Value = 13.17
Minimum Value = 3.20
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
6
8
10
12
Time : 1700 - 1800 LST
Maximum Value = 13.22
Minimum Value = 3.78
4

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)


Time : 1800 - 1900 LST

Maximum Value = 12.74
Minimum Value = 3.72

Time : 1900 - 2000 LST

Maximum Value = 12.27
Minimum Value = 3.53

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
WBH
DKLB
CNYR
MLKM
4
6
8
10
12

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

Appendix F

PERCENT CONTRIBUTION OF INITIAL CONCENTRATIONS, BOUNDARY CONDITIONS (FOUR LATERAL FACES PLUS TOP BOUNDARY) ANTHROPOGENIC AREA SOURCE EMISSIONS, POINT SOURCE EMISSIONS, AND BIOGENIC EMISSIONS TO HOURLY TRACER, NO_x, AND VOC CONCENTRATIONS ON 4 JUNE 1984

F-1a: 0800 Initial NO_x tracer contibution
F-1b: 0800 Boundary NO_x tracer contribution
F-1c: 0800 Area source NO_x tracer contribution
F-1d: 0800 Point source NO_x tracer contribution

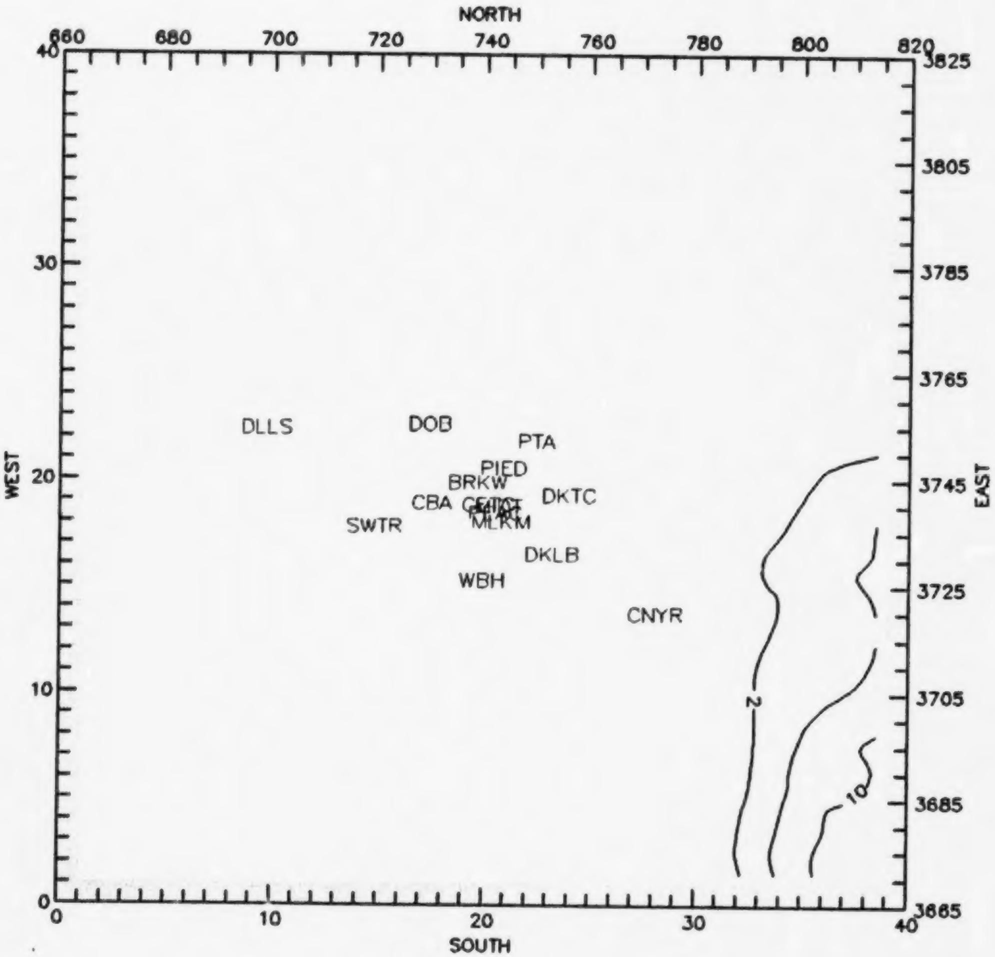
F-2a: 0800 Initial VOC tracer contribution
F-2b: 0800 Boundary VOC tracer contribution
F-2c: 0800 Anthropogenic VOC tracer contribution
F-2d: 0800 Biogenic VOC tracer contribution

F-3a: 1200 Initial NO_x tracer contribution
F-3b: 1200 Boundary NO_x tracer contribution
F-3c: 1200 Area source NO_x tracer contribution
F-3d: 1200 Point source NO_x tracer contribution

F-4a: 1200 Initial VOC tracer contribution
F-4b: 1200 Boundary VOC tracer contribution
F-4c: 1200 Anthropogenic VOC tracer contribution
F-4d: 1200 Biogenic VOC tracer contribution

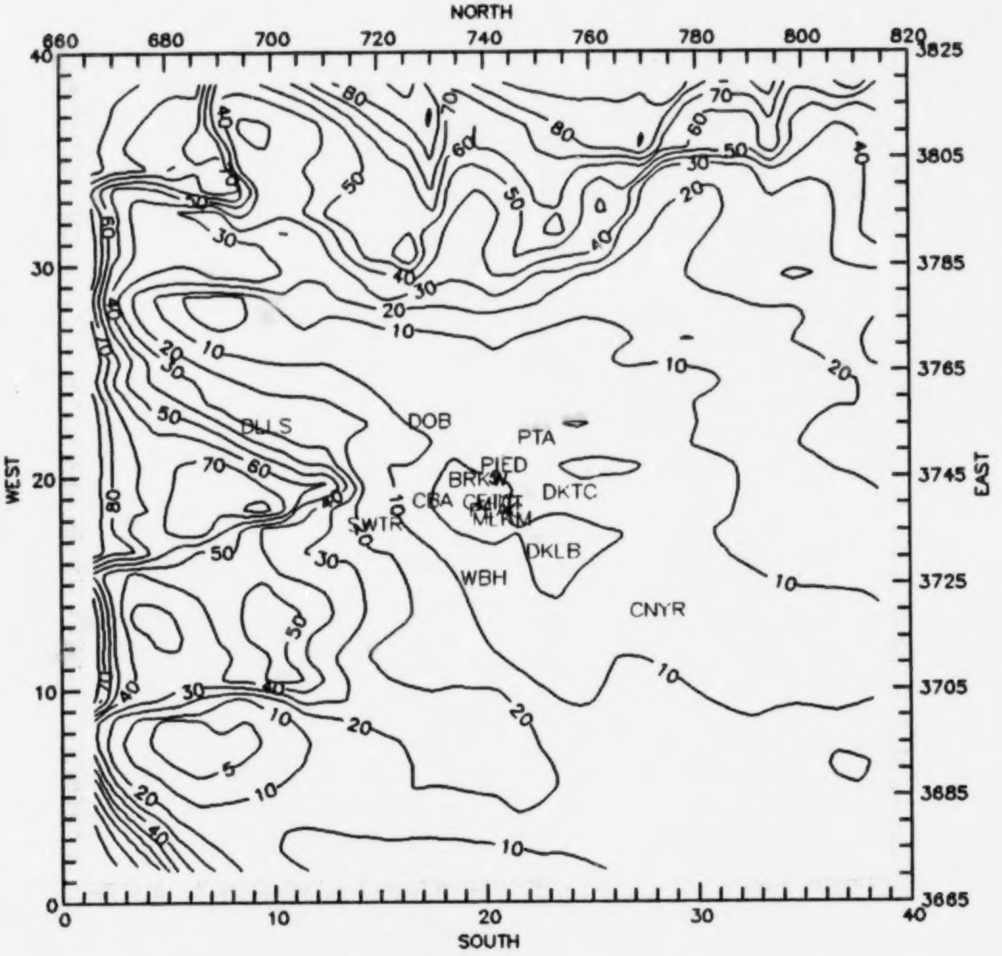
F-5a: 1600 Initial NO_x tracer contibution
F-5b: 1600 Boundary NO_x tracer contribution
F-5c: 1600 Area source NO_x tracer contribution
F-5d: 1600 Point source NO_x tracer contribution

F-6a: 1600 Initial VOC tracer contribution
F-6b: 1600 Boundary VOC tracer contribution
F-6c: 1600 Anthropogenic VOC tracer contribution
F-6d: 1600 Biogenic VOC tracer contribution



NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
EAST
3825
3805
3785
3765
3745
3725
3705
3685
3665
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
2
10

FIGURE **F-1a**. Percent contribution of initial NOx tracer at 800 EST. 4 June 1984.



NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
EAST
3825
3805
3785
3765
3745
3725
3705
3685
3665
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
MLRM
DKLB
SWTR
WBH
CNYR
80
70
60
50
40
30
20
10
5

FIGURE F-1b. Percent contribution of boundary NOx tracer at 800 EST, 4 June 1984.

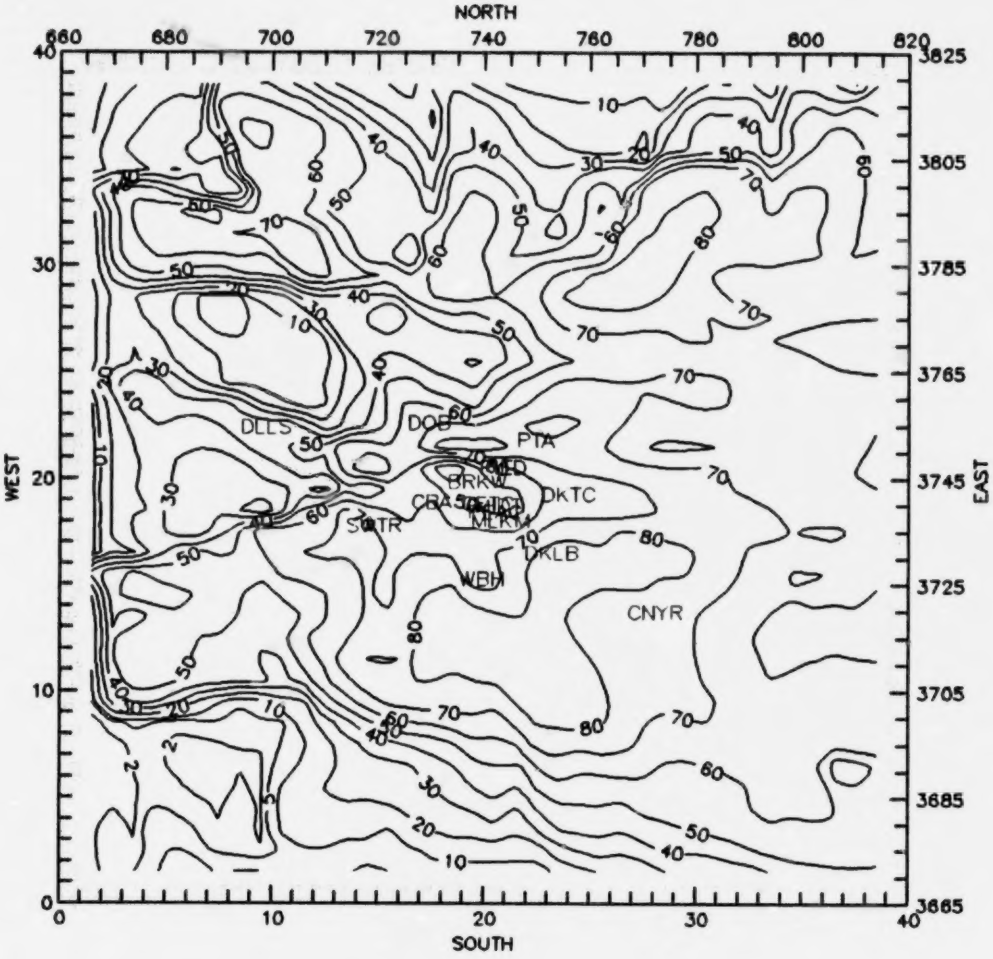

NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
EAST
3825
3805
3785
3765
3745
3725
3705
3685
3665
DLLS
DOB
PTA
BRKW
CBA
DKTC
MLKM
SOTR
DKLB
WBH
CNYR

FIGURE F-1c . Percent contribution of area source NOx tracer at 800 EST, 4 June 1984.

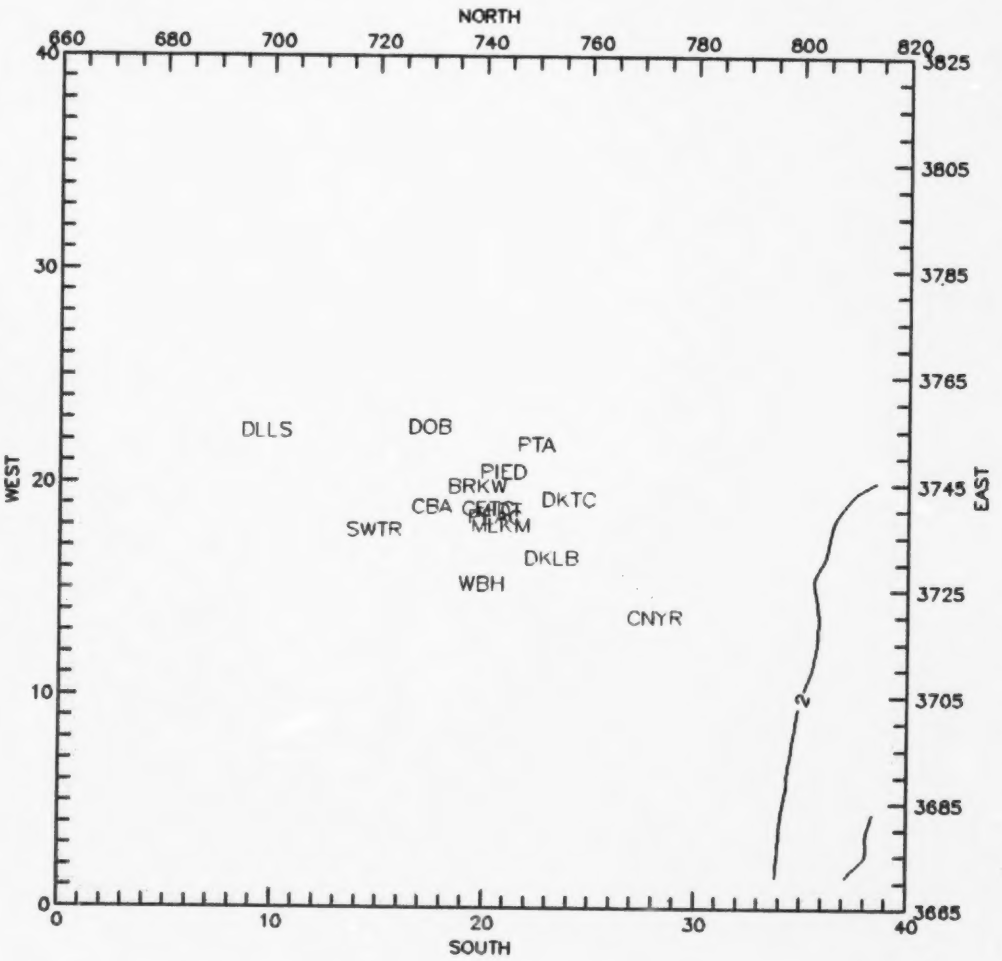

NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
EAST
3825
3805
3785
3765
3745
3725
3705
3685
3665
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
2

FIGURE F-2a . Percent contribution of initial VOC tracer at 800 EST, 4 June 1984.

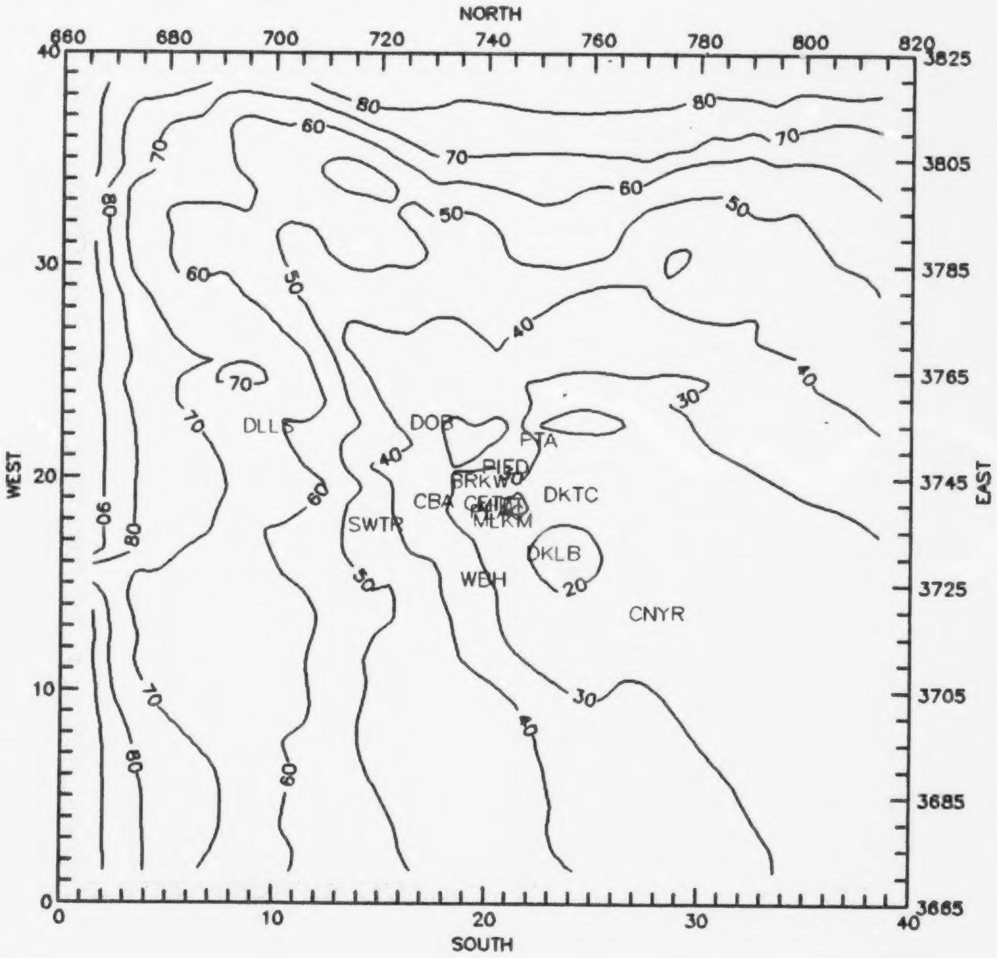

NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
EAST
3825
3805
3785
3765
3745
3725
3705
3685
3665
90
80
70
60
50
40
30
20
DLLS
DOB
PTA
PIED
BRKWO
CEMO
MLKM
CBA
SWTR
DKTC
DKLB
WBH
CNYR

FIGURE F-2b . Percent contribution of boundary VOC tracer at 800 EST, 24 June 1984.

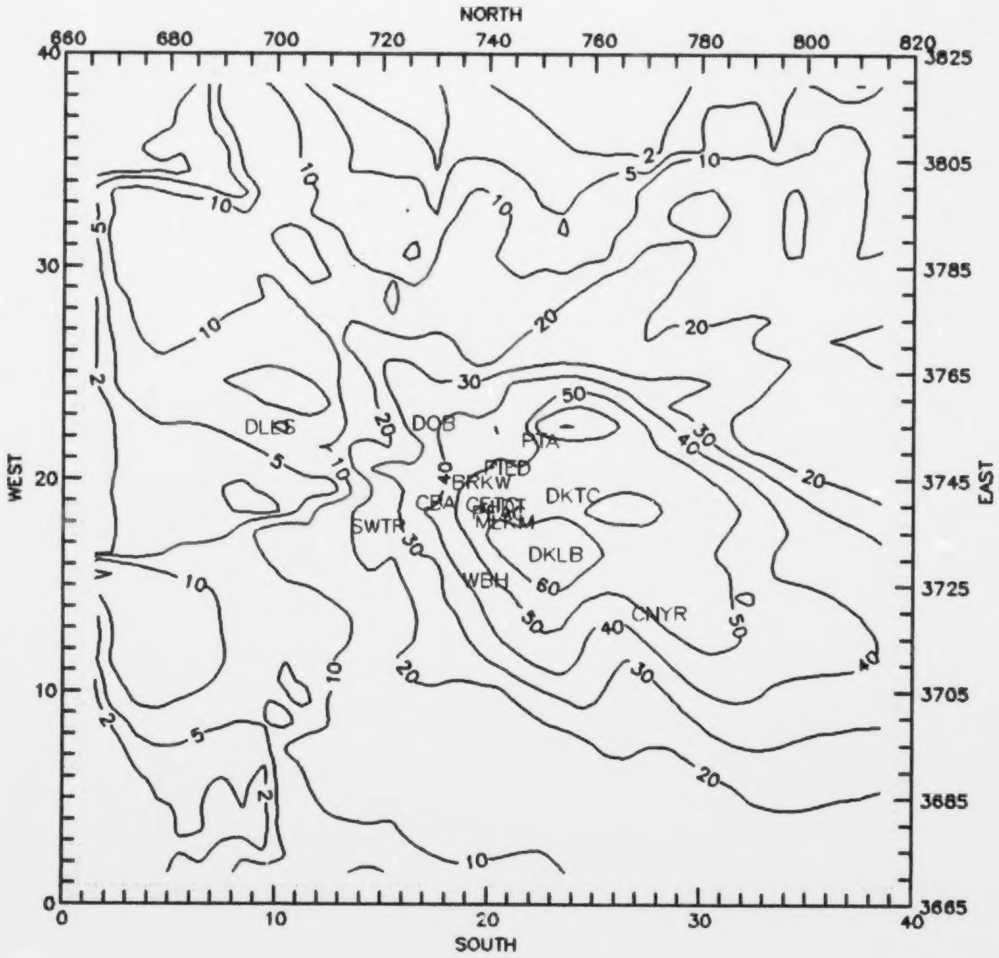

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLKS
DOB
PTA
PTED
BRKW
CBA
DKTC
DKLB
SWTR
WBH
CNYR
2
5
10
20
30
40
50
60

FIGURE F-2c. Percent contribution of anthropogenic VOC tracer at 800 EST, 4 June 1984.

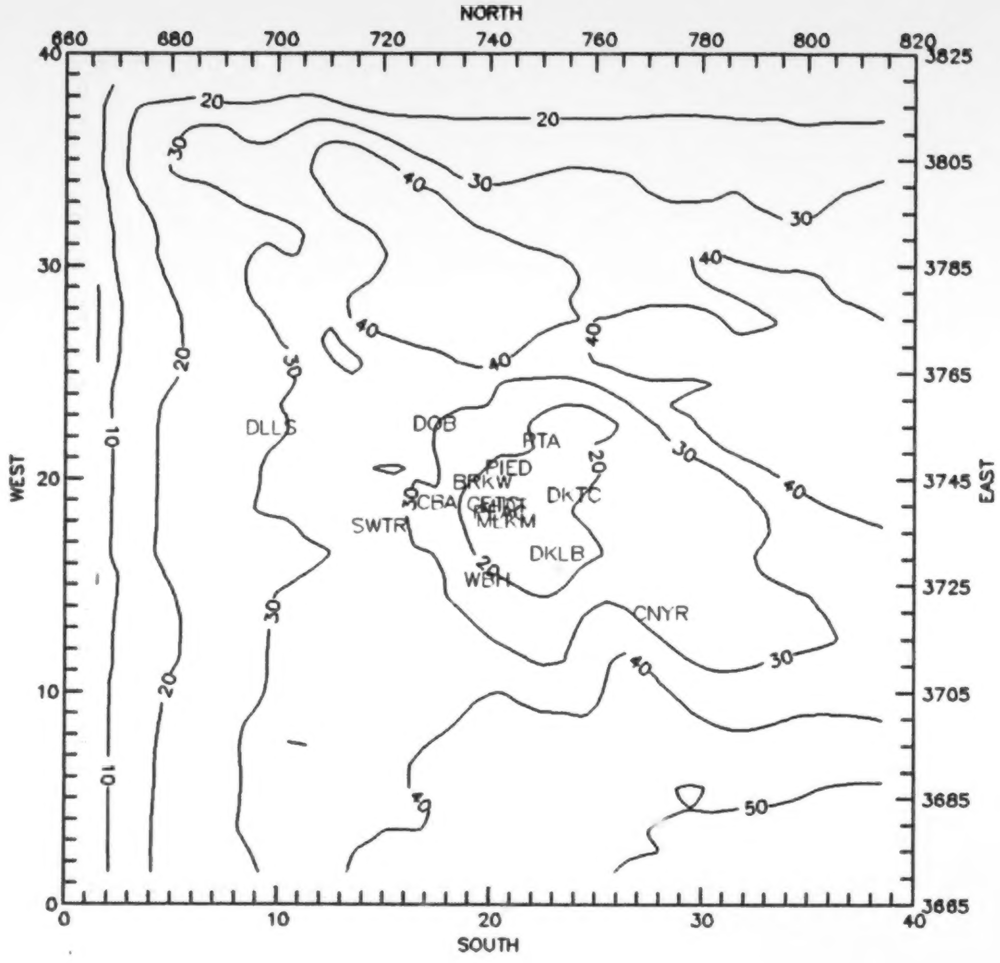
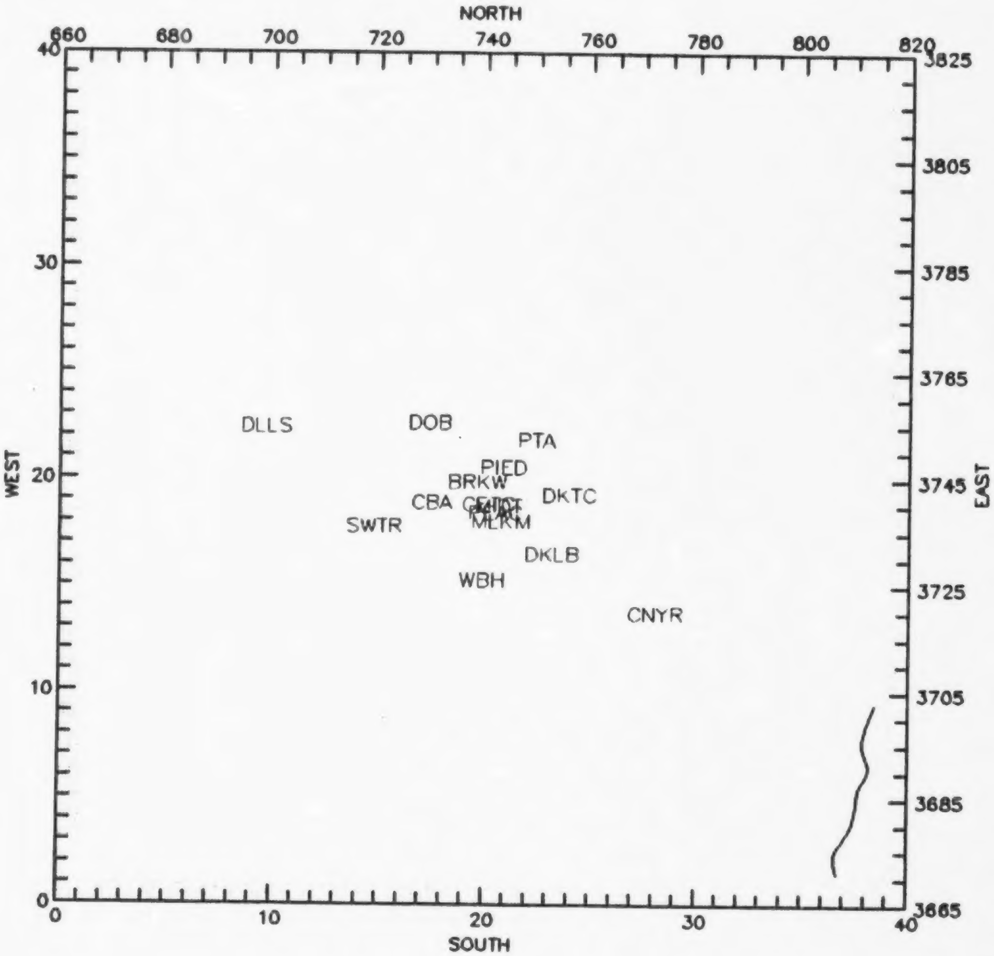

NORTH
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
EAST
WEST
40
30
20
10
0
SOUTH
10
20
30
40
DLLS
DOB
RTA
PIED
BRKW
DKTC
CBA
MLKM
SWTR
DKLB
WEH
CNYR
50

FIGURE F-2d . Percent contribution of biogenic VOC tracer at 800 EST, 4 June 1984.



NORTH
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
EAST
40
30
20
10
0
WEST
0
10
20
30
40
SOUTH
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR

FIGURE F-3a . Percent contribution of initial NOx tracer at 1200 EST. 4 June 1984.

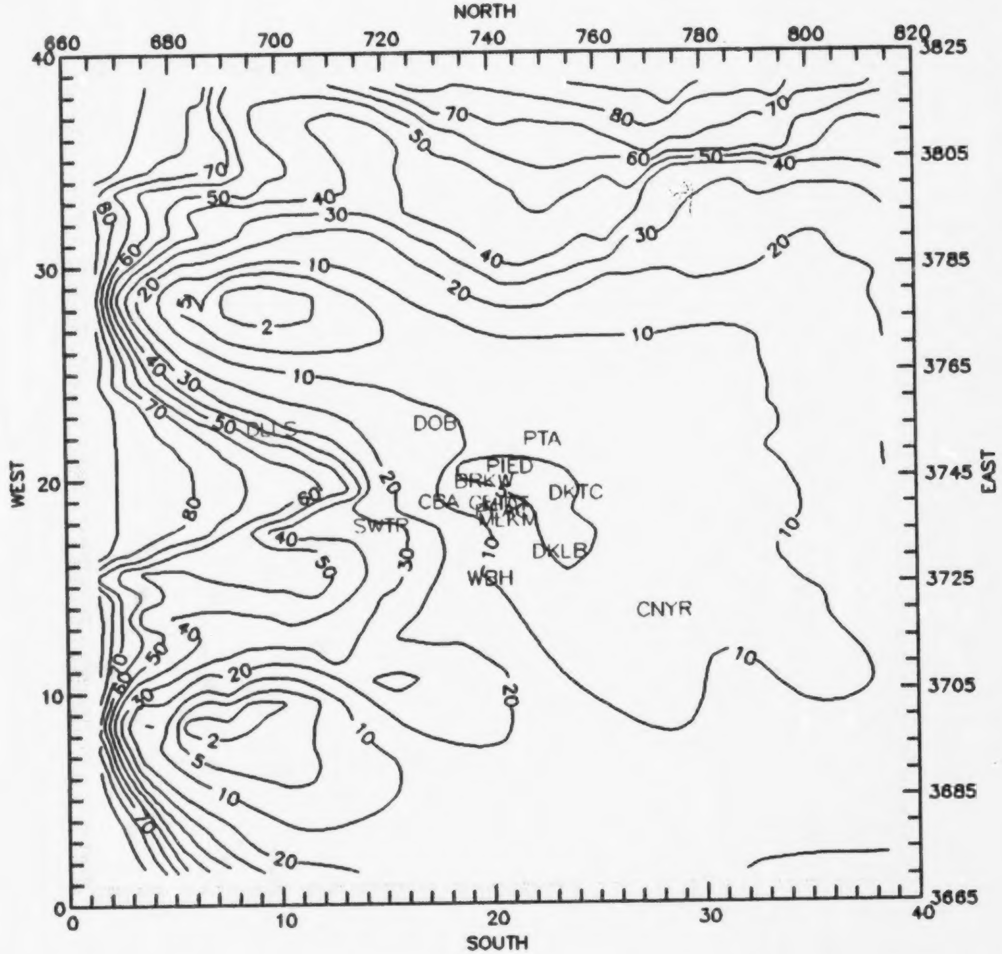

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
0
10
20
30
40
3825
3805
3785
3765
3745
3725
3705
3685
3665
DOB
PTA
PIED
BRKW
CBA
DKTC
DKLB
WBH
SWTR
DLLS
CNYR
2
5
10
20
30
40
50
60
70
80

FIGURE F-3b. Percent contribution of boundary NOx tracer at 1200 EST, 4 June 1984.

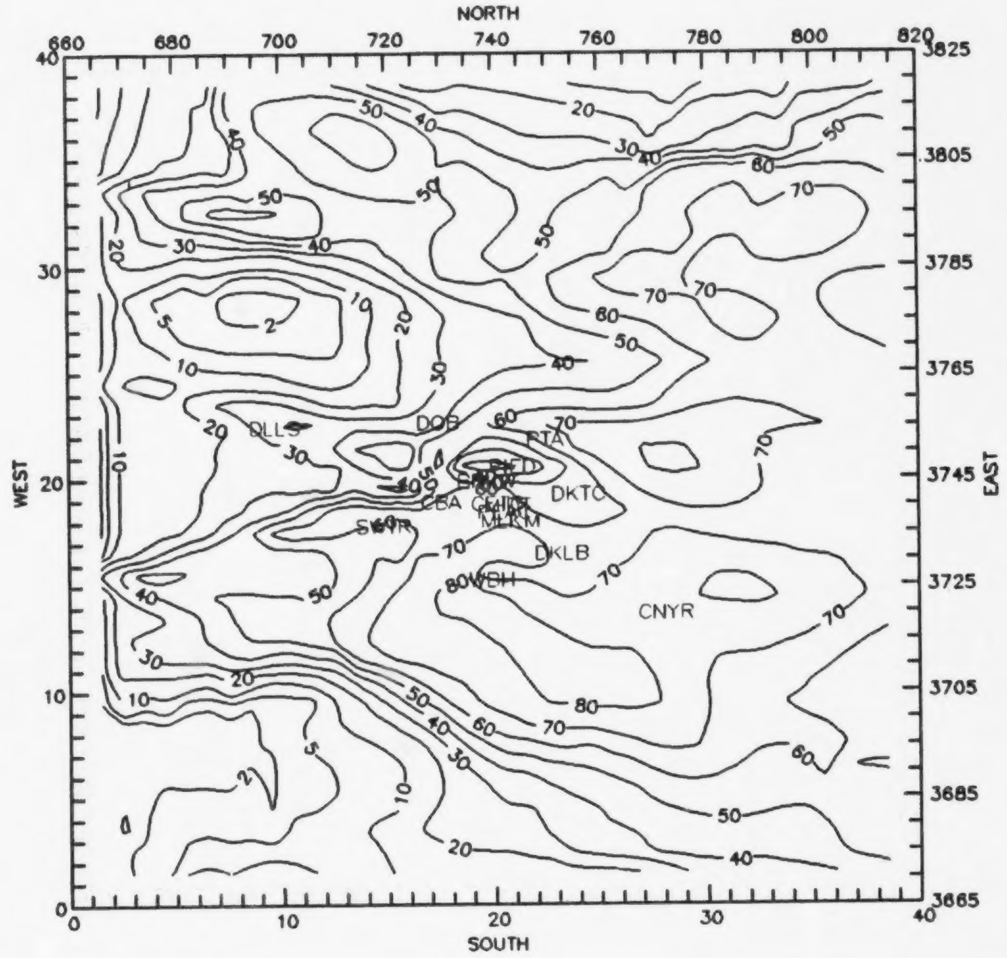

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
DKTC
CBA
MLKM
SKYR
DKLB
BWBH
CNYR

FIGURE F-3c . Percent contribution of area source NOx tracer at 1200 EST, 4 June 1984.

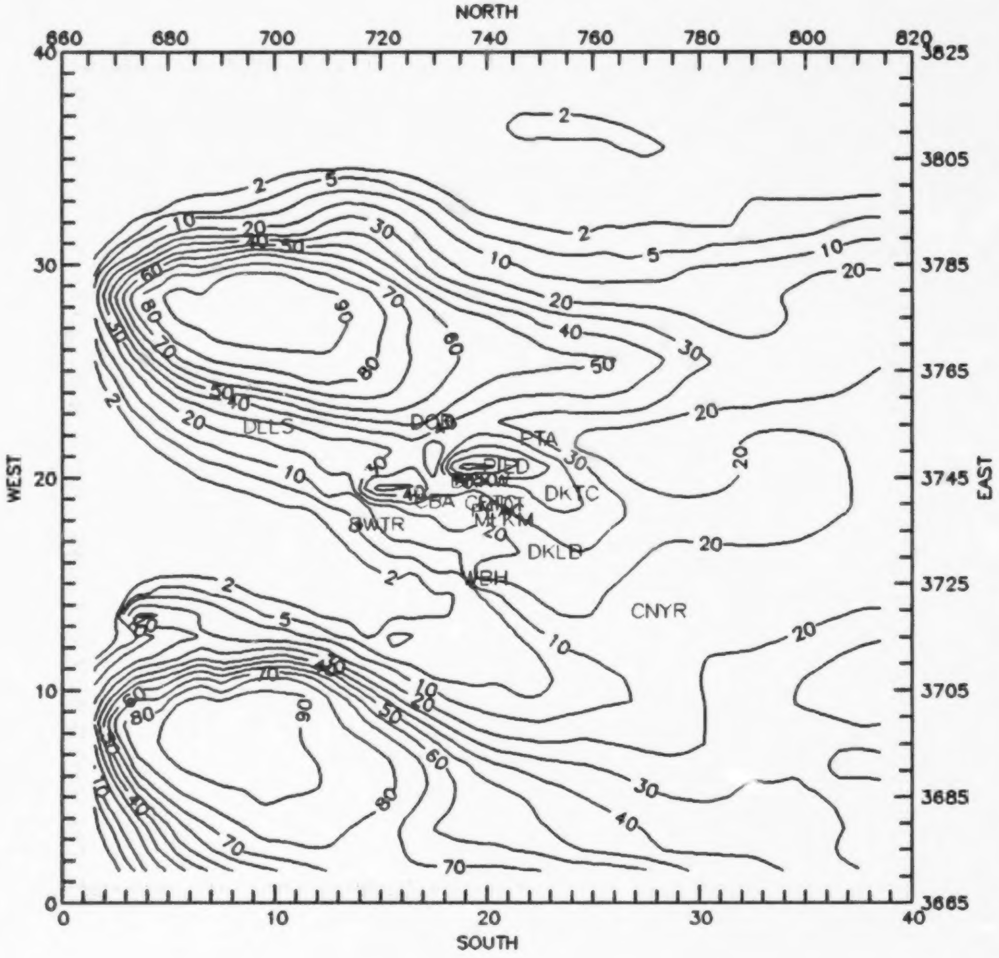

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PLLD
DKTC
CBA
MLKM
SWTR
DKLB
WBH
CNYR

FIGURE F-3d. Percent contribution of point source NOx tracer at 1200 EST. 4 June 1984.

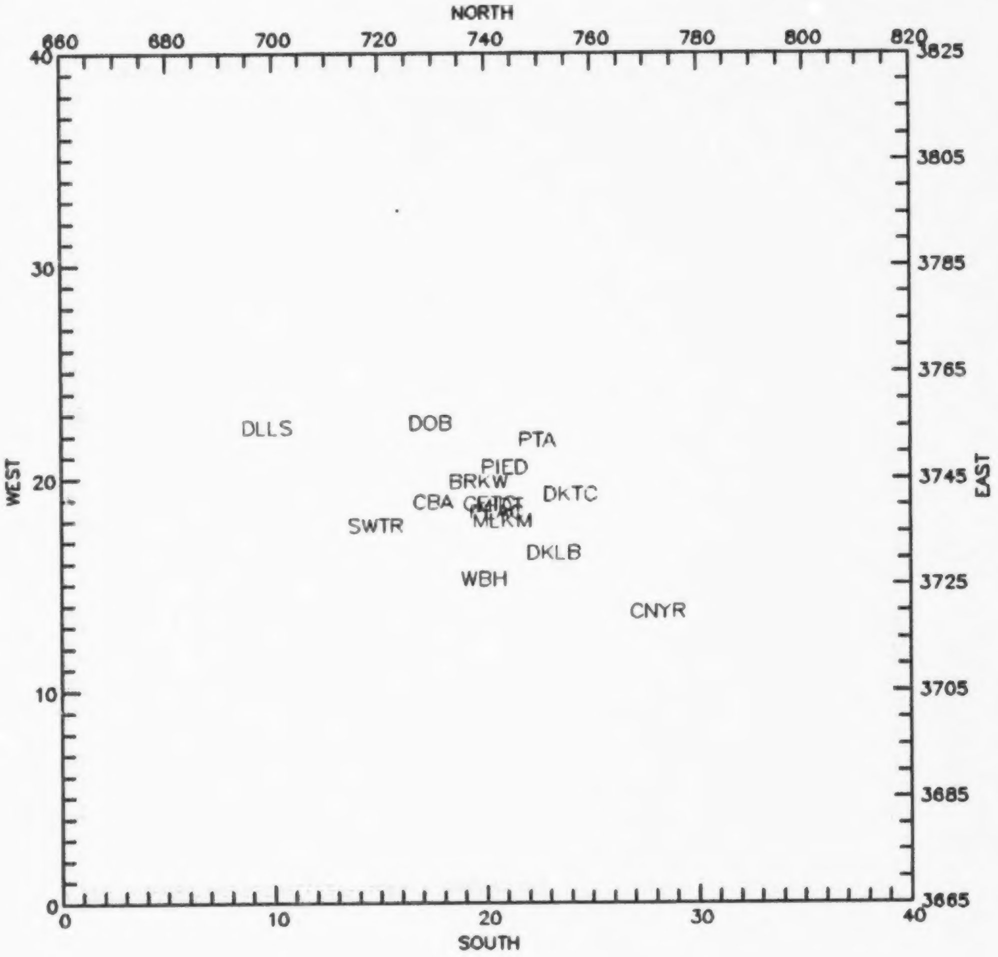

NORTH
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
EAST
WEST
40
30
20
10
0
SOUTH
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR

FIGURE **F-4a**. Percent contribution of initial VOC tracer at 1200 EST. 4 June 1984.

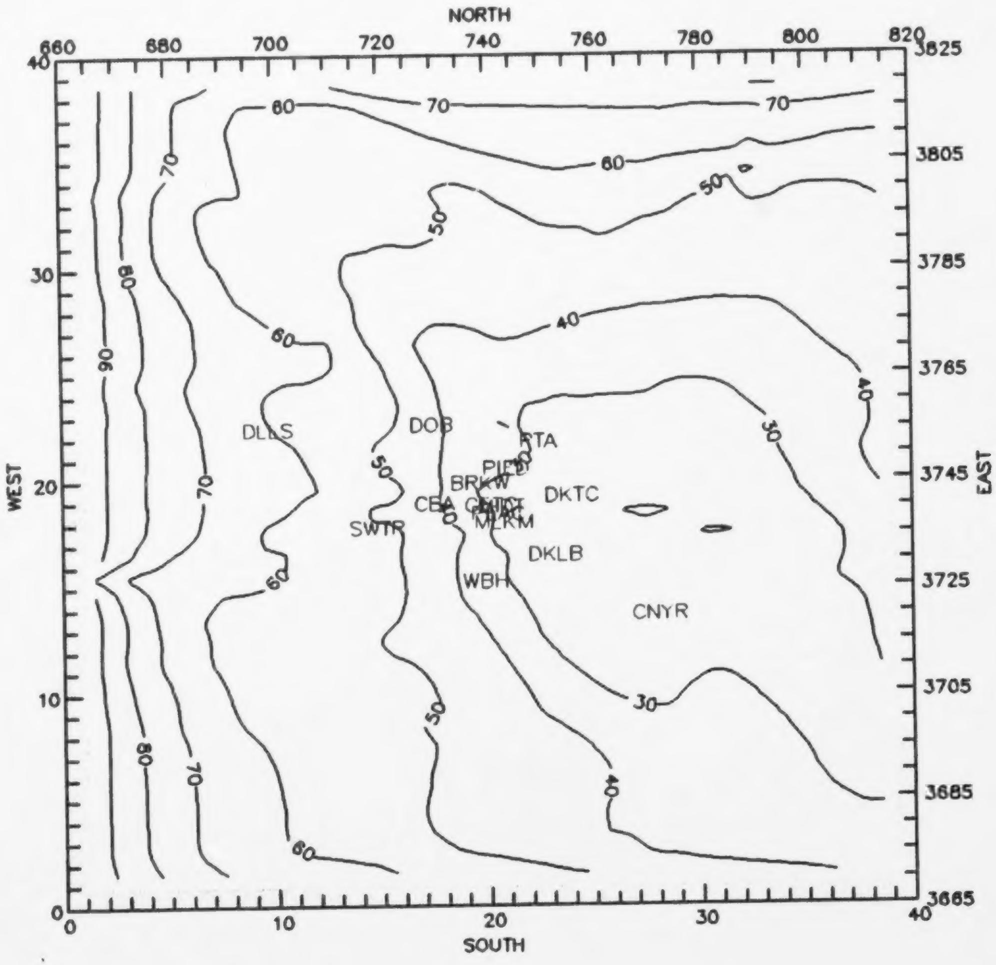

NORTH
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
EAST
WEST
40
30
20
10
0
SOUTH
0
10
20
30
40
90
80
70
60
50
40
30
DLLS
DOB
RTA
PIED
BRKW
CBA
MLRM
SWTR
DKTC
DKLB
WBH
CNYR

FIGURE F-4b . Percent contribution of boundary VOC tracer at 1200 EST, 4 June 1984.

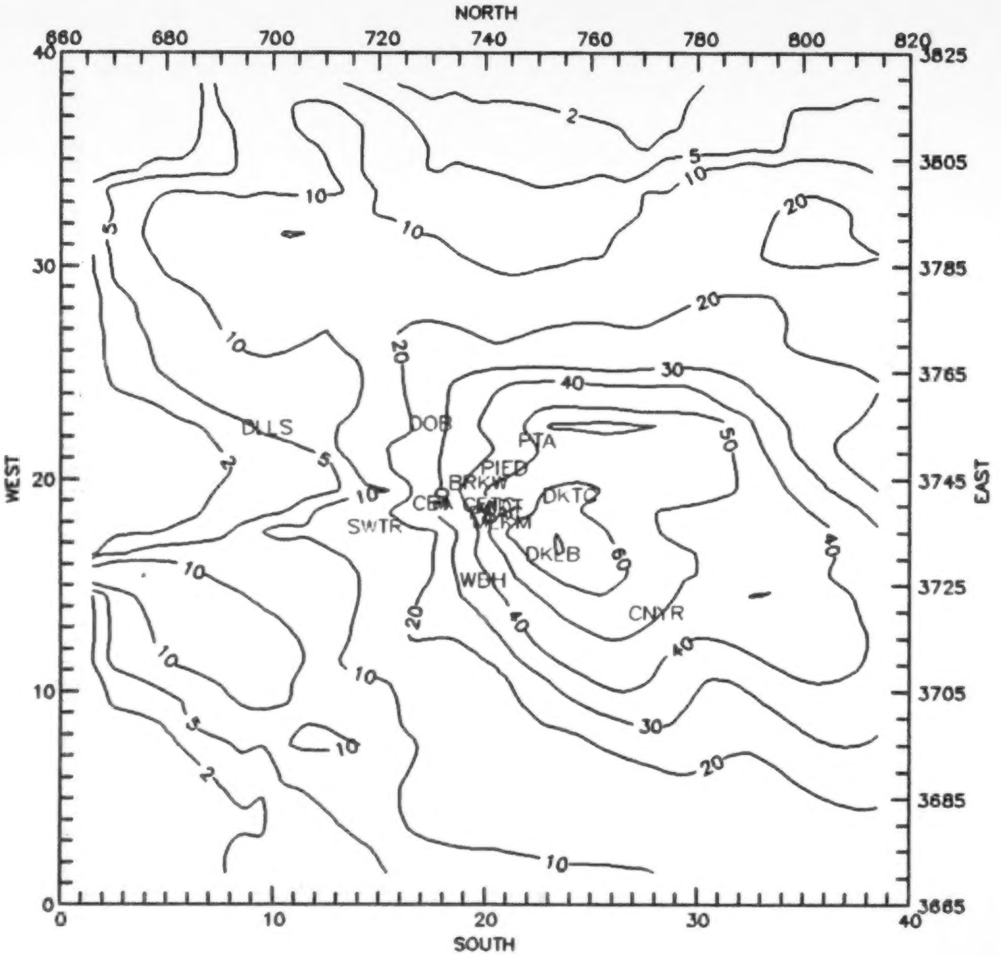

NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
EAST
3825
3805
3785
3765
3745
3725
3705
3685
3665
2
5
10
20
30
40
50
60
DLLS
SWTR
DOB
CBA
BRKW
PIED
PTA
DKTC
WERM
DKLB
WBH
CNYR

FIGURE F-4c. Percent contribution of anthropogenic VOC tracer at 1200 EST, 4 June 1984.

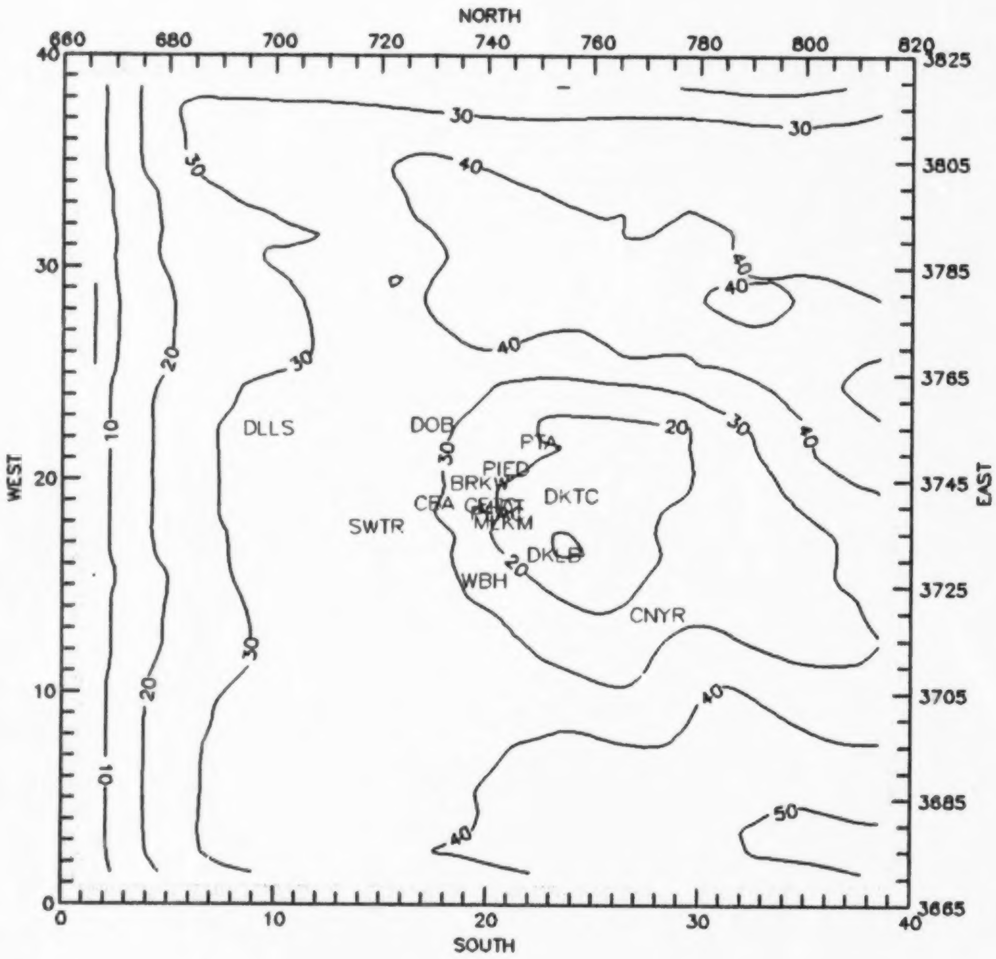

NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
0
10
20
30
40
EAST
3665
3685
3705
3725
3745
3765
3785
3805
3825
10
20
30
40
50
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR

FIGURE **F-4d**. Percent contribution of biogenic VOC tracer at 1200 EST, 24 June 1984.

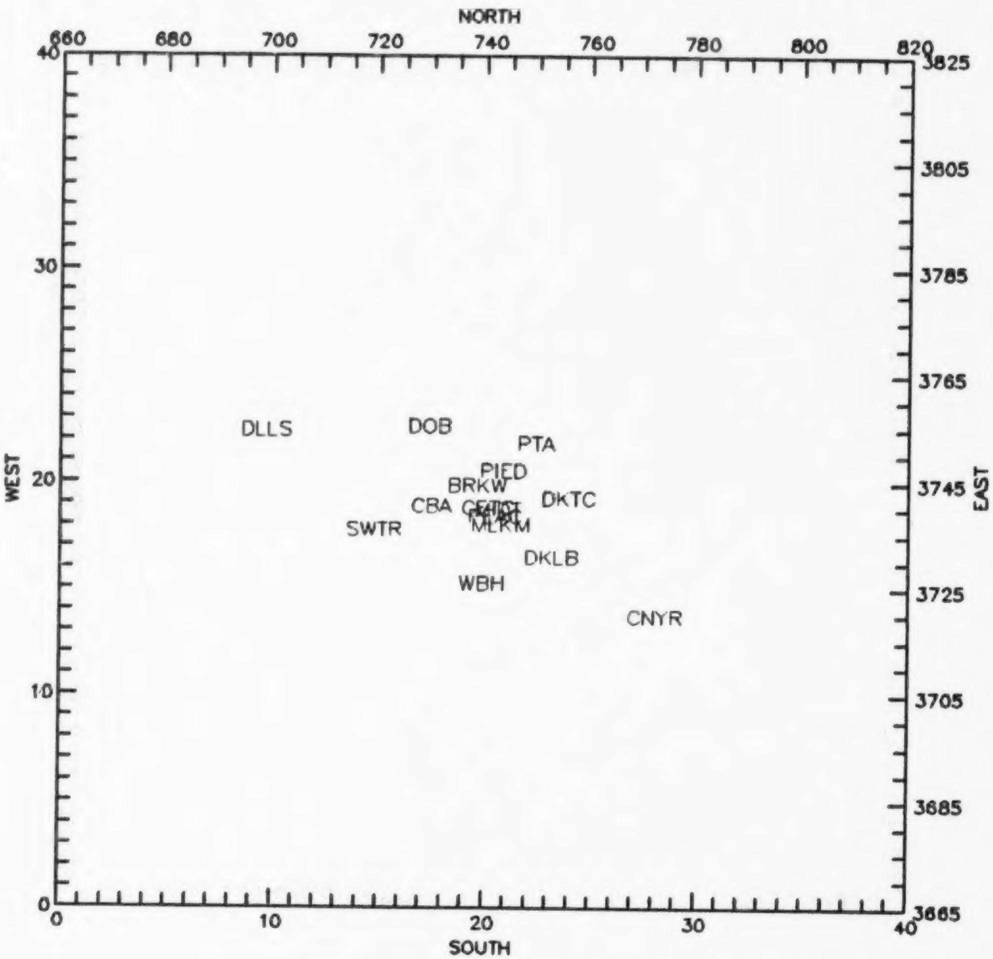


FIGURE F-5a. Percent contribution of initial NOx tracer at 1600 EST, 4 June 1984.

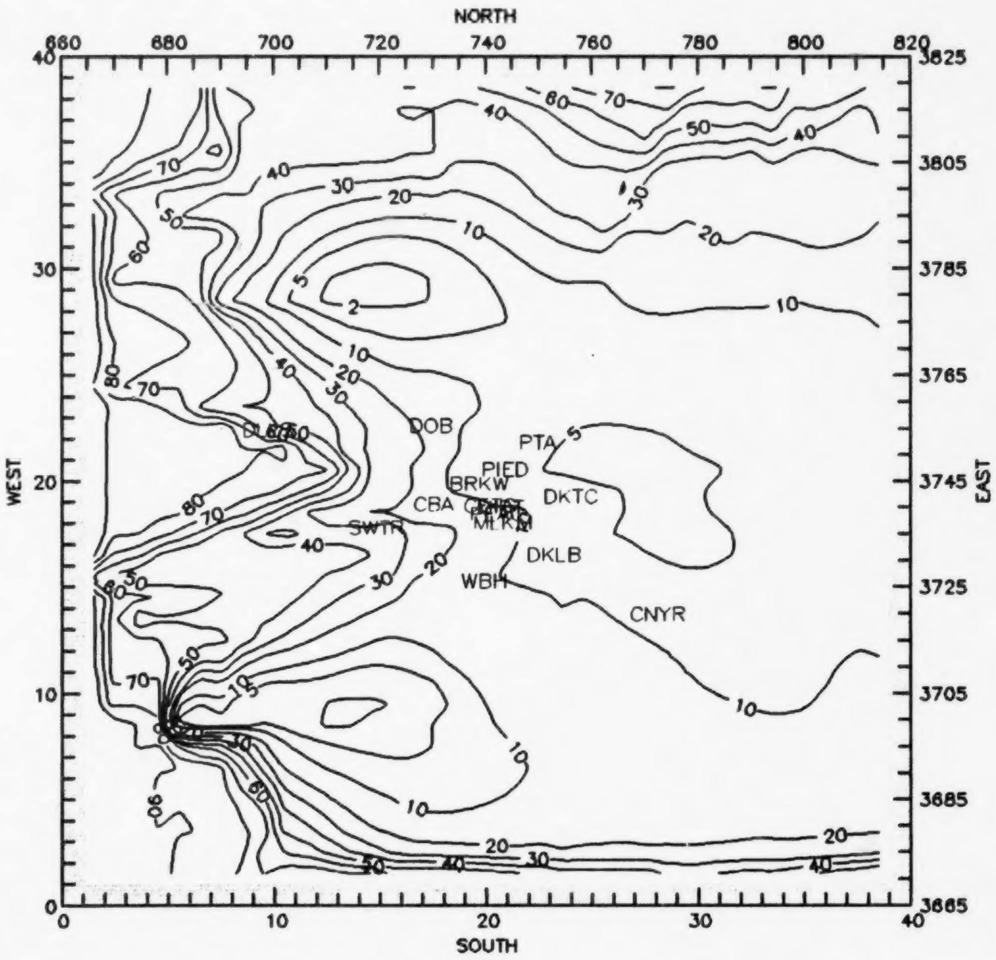

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
0
10
20
30
40
3665
3685
3705
3725
3745
3765
3785
3805
3825
DOB
PTA
PIED
BRKW
DKTC
CBA
SWTR
MLK
DKLB
WBH
CNYR
2
5
10
20
30
40
50
60
70
80
90

FIGURE **F-5b** . Percent contribution of boundary NOx tracer at 1600 EST, 4 June 1984.

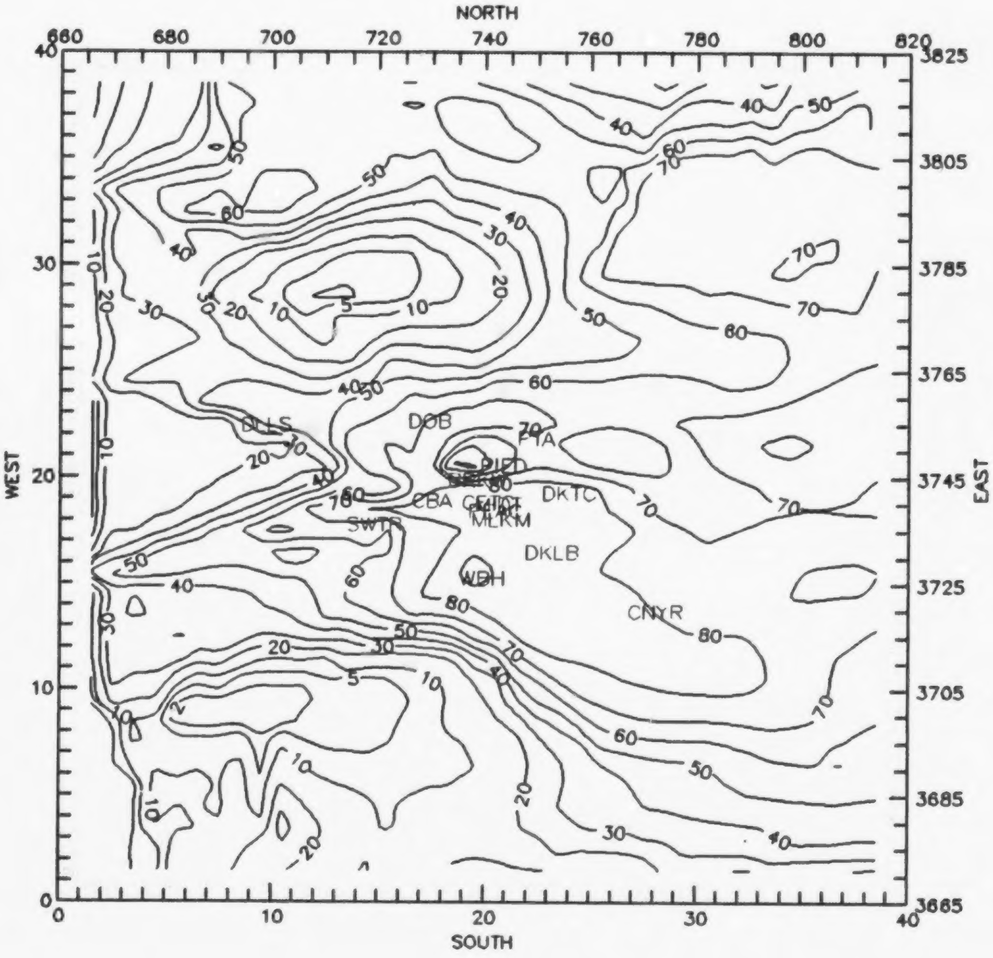

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
FTA
PIED
DKTC
CBA
MLKM
SWTR
DKLB
WBH
CNYR

FIGURE F-5c . Percent contribution of area source NOx tracer at 1600 EST, 4 June 1984.

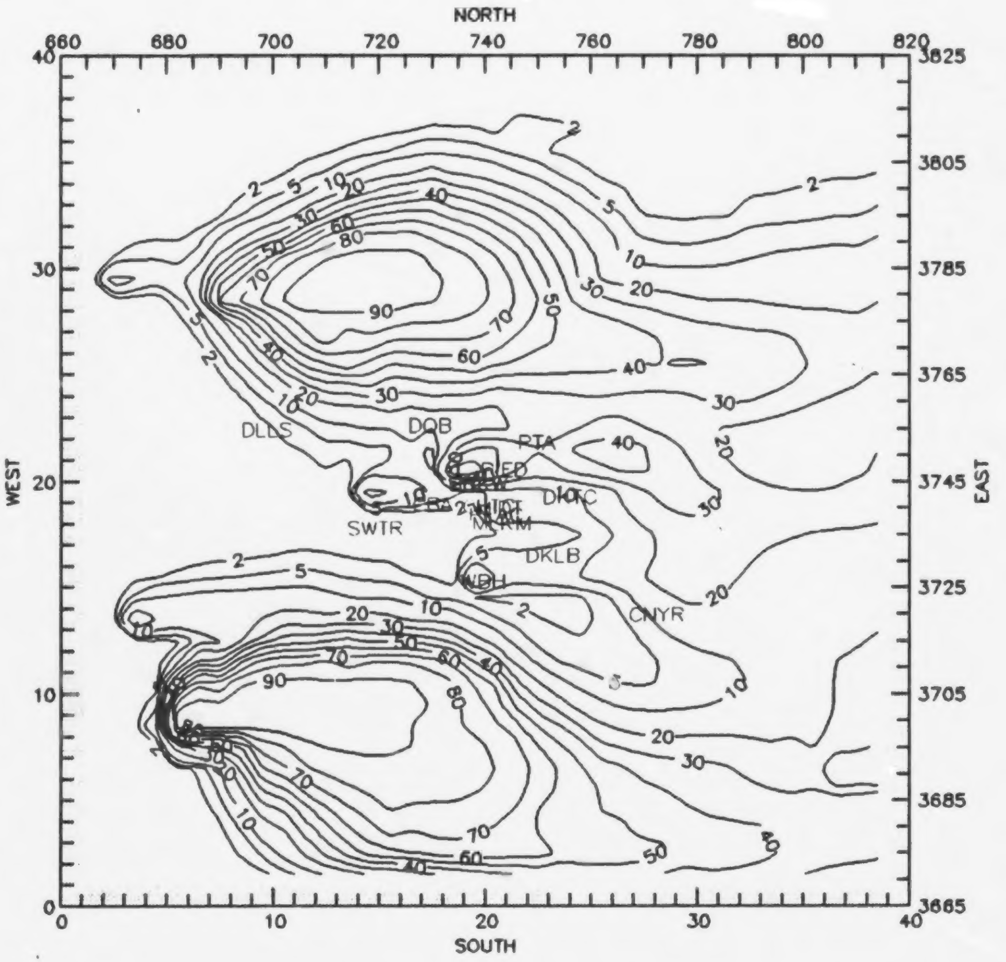

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
DKTC
SWTR
DKLB
WDH
CNYR
2
5
10
20
30
40
50
60
70
80
90

FIGURE F-5d . Percent contribution of point source NOx tracer at 1600 EST, 4 June 1984.

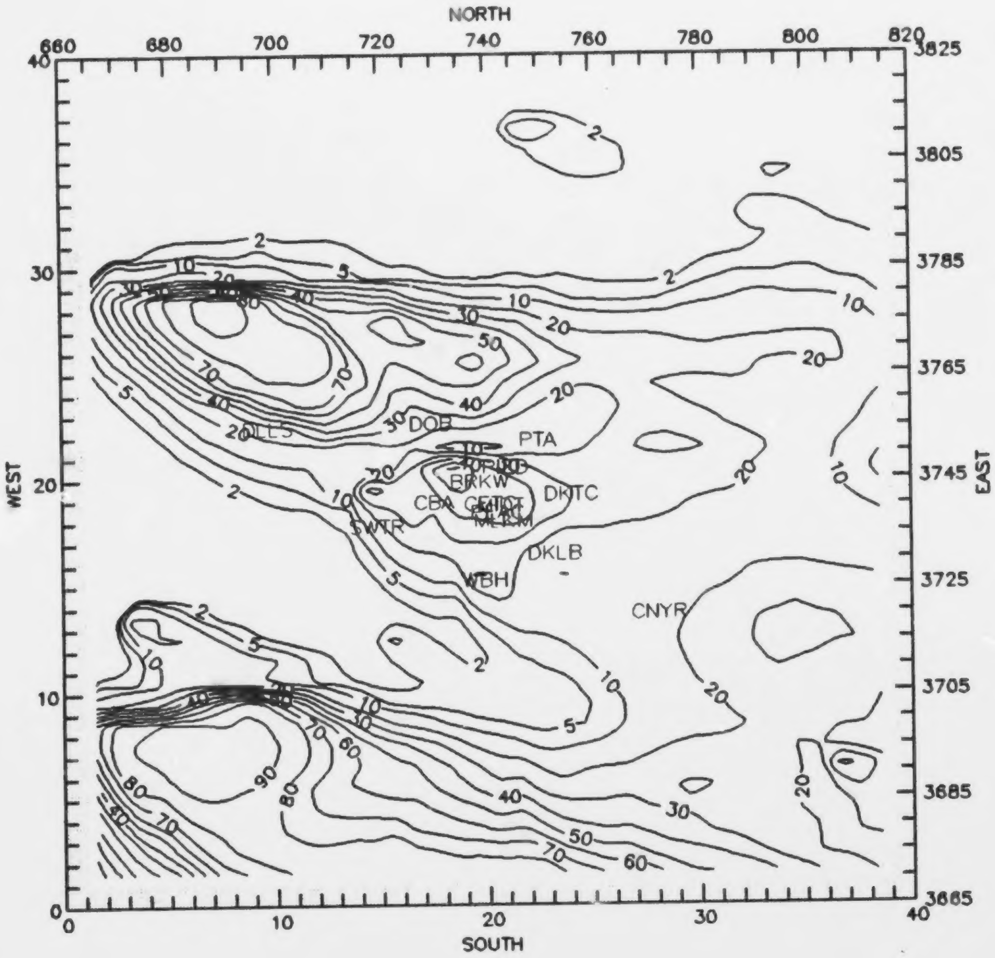

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DOB
PTA
BRKW
CBA
DKTC
SWTR
DKLB
WBH
CNYR
DLLS
2
5
10
20
30
40
50
60
70
80
90

FIGURE F-1d. Percent contribution of point source NOx tracer at 800 EST, 4 June 1984.

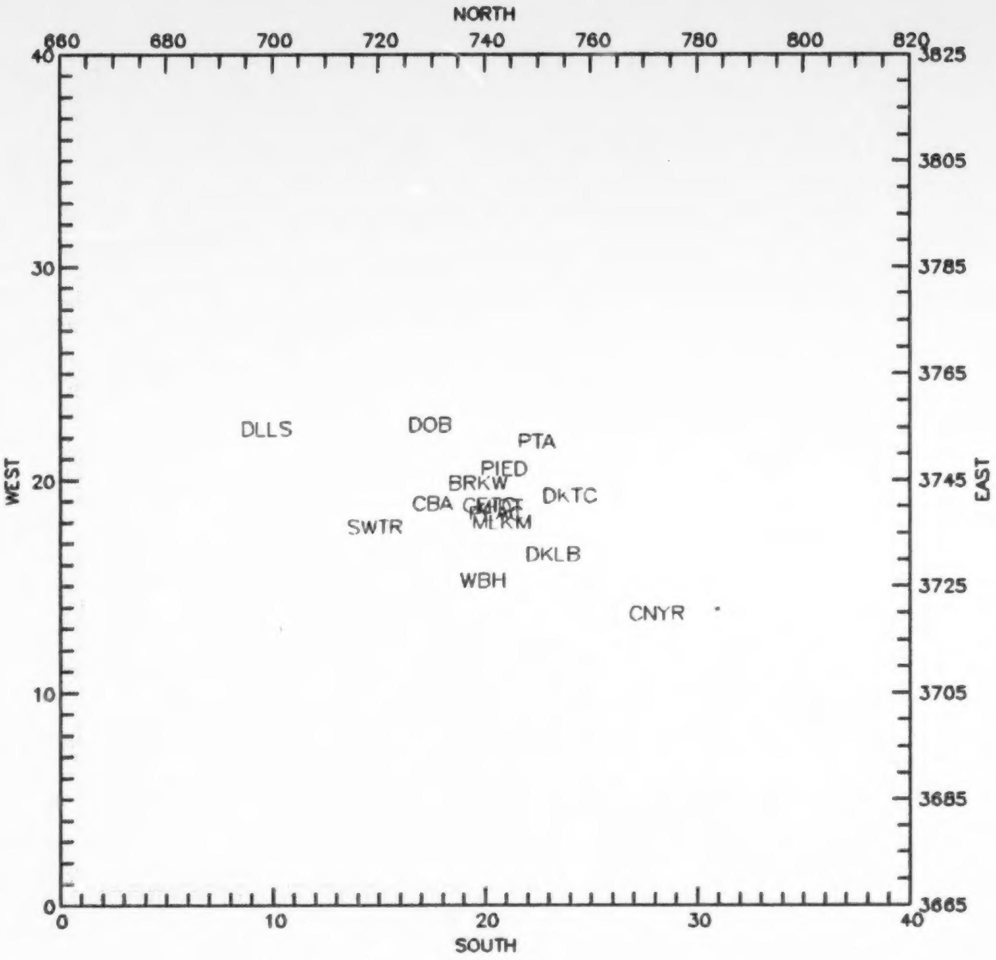


FIGURE F-6a . Percent contribution of initial VOC tracer at 1600 EST. 4 June 1984.

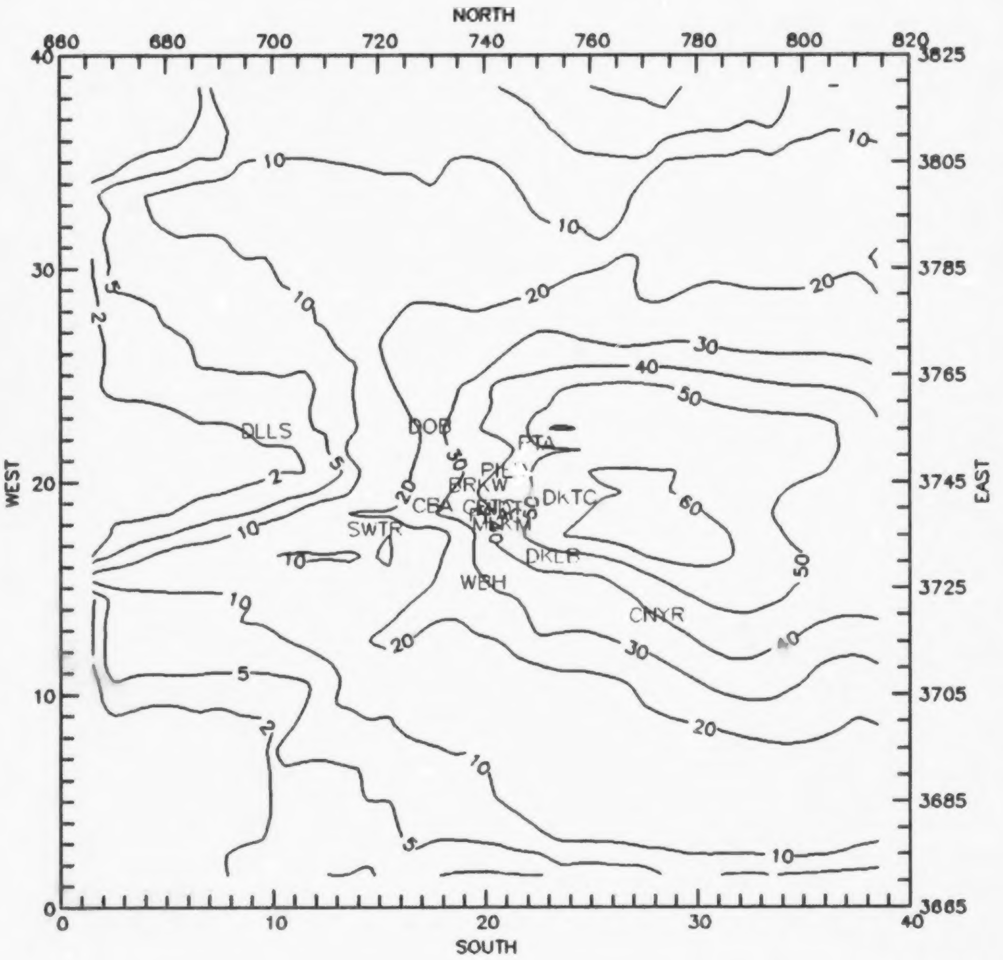

NORTH
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
EAST
WEST
40
30
20
10
0
0
10
20
30
40
SOUTH
DLLS
DOB
PTA
PIL
BRKW
CBA
DKTC
SWTR
MBRM
DKLR
WBH
CNYR
2
5
10
20
30
40
50
60

FIGURE **F-6b**. Percent contribution of anthropogenic VOC tracer at 1600 EST. 4 June 1984.

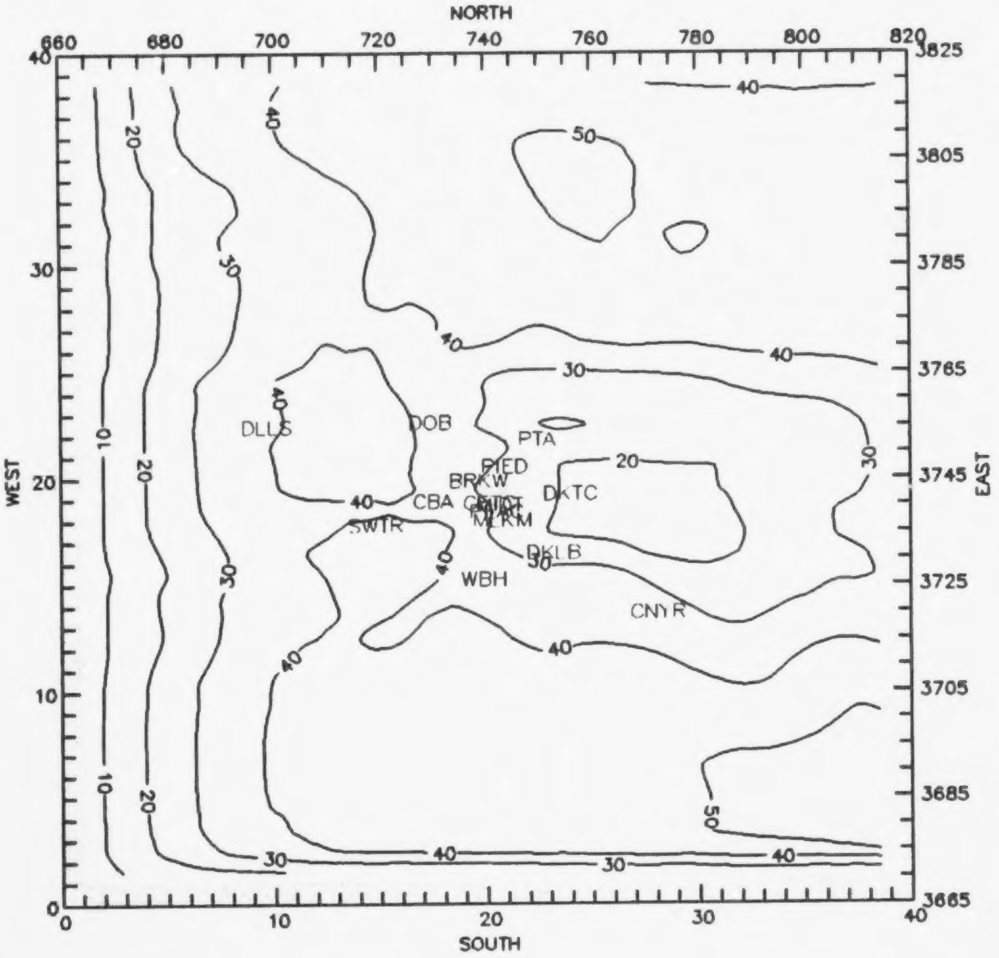


FIGURE F-6c. Percent contribution of biogenic VOC tracer at 1600 EST, 24 June 1984.

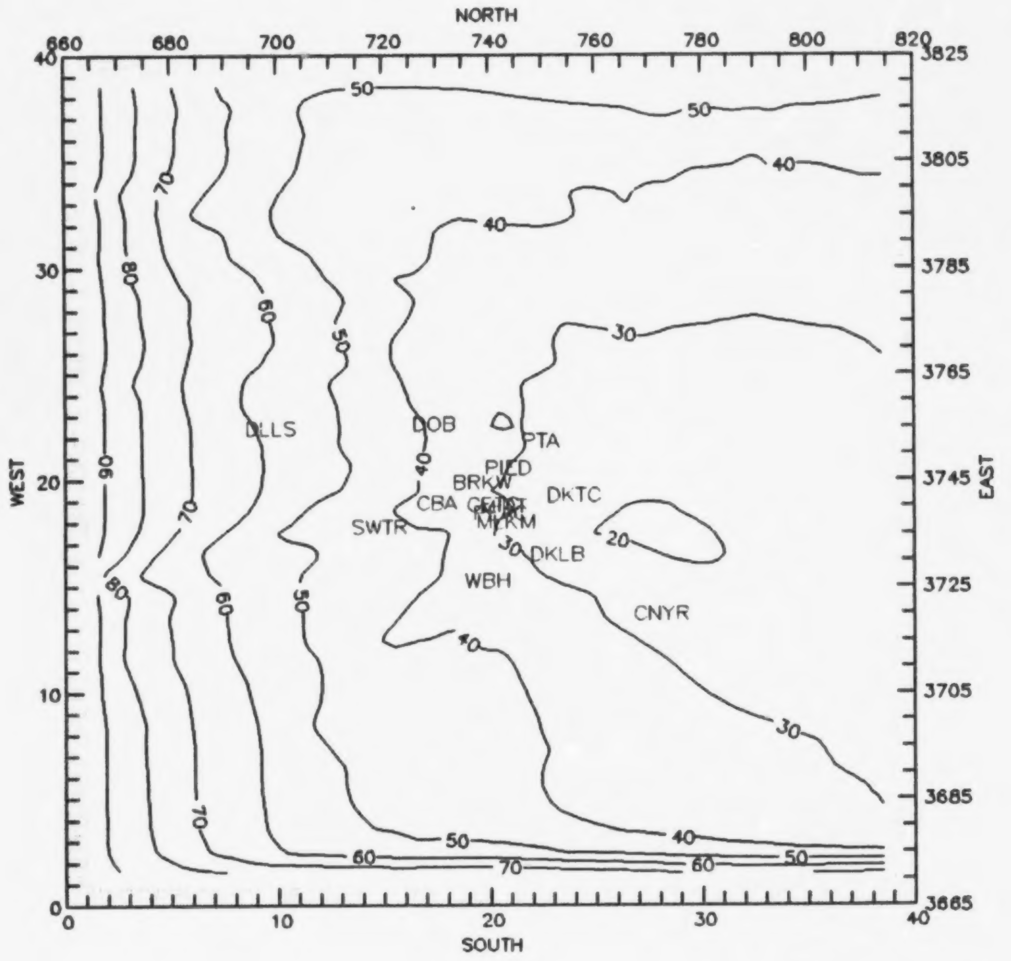

NORTH
660
680
700
720
740
760
780
800
820
SOUTH
0
10
20
30
40
WEST
EAST
3825
3805
3785
3765
3745
3725
3705
3685
3665
90
80
70
60
50
40
30
20
DLLS
DOB
PTA
PIED
BRKW
DKTC
CBA
SWTR
MLKM
DKLB
WBH
CNYR

FIGURE F-6d. Percent contribution of boundary VOC tracer at 1600 EST, 4 June 1984.

Appendix G

SENSITIVITY ANALYSIS OF THE CALCULATIONS OF OZONE CONCENTRATIONS AND EFFECTS OF EMISSION CONTROLS ON OZONE CONCENTRATIONS TO WIND SPEED SPECIFICATION

Appendix G

SENSITIVITY ANALYSIS OF THE CALCULATIONS OF OZONE CONCENTRATIONS AND EFFECTS OF EMISSION CONTROLS ON OZONE CONCENTRATIONS TO WIND SPEED SPECIFICATION

Because of the limited air quality and meteorological monitoring data in the vicinity of Atlanta there is some question whether the base case UAM simulation is simulating all of the pertinent physical, meteorological, and chemical processes that led to the high ozone episode of 4 June, 1984. The only indication of whether the model is correctly simulation such an episode is its ability to predict the hourly ozone concentrations at the three ozone monitoring sites. The base case modeling inputs from evaluation run 2 exhibited model performance that barely passed the model performance goal. There were several explanations given for the descrepencies between the predicted and observed ozone concentrations including: underestimation of the anthropogenic emissions inventory; use of too low boundary conditions; excessive wind shear which tended to dilute the urban plume; and excessive wind speads which also tended to dilute the urban plume. Thus it was decided to do a sensitivity test which would result in less dilution of the urban plume. This was accomplished by reducing the wind speeds at all FAA wind observations sites by 50 percent.

The justification of this wind speed reduction is based on the instanteneous nature of the observed FAA wind speeds versus the hourly integrated wind speeds required by the UAM and the bias in the human FAA observations versus the mechanical wind averaging techniques. When there is wind variations throughout the hour, then the vector averaging of the hourly average wind speeds will result in a lower value than reported at an FAA site, which is essential an instantenous value taken at the end of an hour. In addition, the human element and uses of the FAA wind speeds are different then the wind information required by the UAM. An important use of the FAA wind observations is their use to advise pilots of adverse wind conditions at the airport for takeoffs and landings. During slow wind conditions, as typically occurs during an ozone episode, the FAA observer may report higher wind gusts that will affect an aircraft operation. The fact that the hourly average wind speed is calm is of no use to the pilot. This bias of FAA wind speeds was noted while developing UAM inputs for the California South Coast Air Basin where there were several hourly integrated and FAA wind observation sites located in the proximity to each other. A brief analysis of these sites is reported next.

COMPARISON OF HOURLY AVERAGED AND FAA WIND SPEED OBSERVATIONS

During the development of the California South Coast Air Basin (SCAB) Air Quality Management Plan (AQMP) study in which four 3-day episodes of high ozone days were extensively studied, a systematic bias was seen between the 1-hour vector averaged SCAQMD (South Coast Air Quality Management District) surface wind speed monitors observations and nearby 1-min averaged NWS/FAA (National Weather Service/ Federal Aviation Administration) observations of surface wind speed. To estimate the extent of the bias seven "collocated" station pairs of NWS/FAA stations with SCAQMD wind monitors were studied. Table G-1 shows the station pairs and the distance between the collocated pairs.

The study periods were the high ozone episodes of 5-7 June, 12-14 August, 21-23 August and 26-28 August 1985. A total of 1920 collocated observation data points were collected. This set was reduced by 801 data points because of either a missing station pair or a station pair that was below the speed of 1 knot. The speed of 1 knot represents the lowest value that FAA/NWS wind monitoring stations can measure thus comparison between SCAQMD stations reporting wind speeds as low as 0.1 mph might introduce a bias towards higher values being reported for FAA/NWS stations.

The mean value for the remaining 1119 data points for the FAA/NWS stations was 3.49 m/s while the mean for the SCAQMD stations was 1.93 m/s suggesting that the FAA/NWS stations were biased by approximately 45 percent (i.e. the observed hourly average wind speeds were a lttle over half of the FAA wind observations). The median values were very similar with values of 3.10 m/s for FAA/NWS stations and 1.80 m/s for SCAQMD stations. Each day was examined to see if any particular day showed an extreme bias, the bias ranged from 36 percent on 13 August to 51 percent on 26 August.

Similarly, all seven stations were examined to see if any particular station may have been the cause of the bias. Five of the seven stations showed similar bias ranging from 45 to 56 percent. However, two pairs showed a significantly smaller bias, the Upland and Ontario airport showed a bias of only 28.8 percent and the San Bernadino and Norton Air Force Base pair showed a bias of only 2.4 percent. In an attempt to see if the agreement was caused by low wind speeds at Norton Air Force Base at night the wind observations were stratified into a daytime period only, we still found that almost no bias occurred for the San Bernadino-Norton Air Force pair. The possibility exists that the data may have been incorrectly processed or reported; if the data was incorrectly converted from knots to m/s this may have account for the small bias.

We believe that the wind speeds reported for 1-minute averages from FAA/NWS stations are correct, however what is needed for the UAM is the 1-hour vector averaged wind speed. As a result of the SCAQMD study, which should be true for all locations in the United States, it was concluded that FAA/NWS surface wind observations have a positive bias of about a factor of 2 and should be reduced by approximately 50 to 75 percent when hourly average wind speeds are desired.

This preliminary analysis is by no means complete or statistically roboust, however it does have important implications in the development of wind fields for air quality simulations models such as the UAM. It also helps explain some underprediction tendency (e.g. St. Louis and Philadelphia) of the UAM at some locations in the past. Further analysis of the SCAQMD wind data base and data from other locations is necessary to determine the extent and frequency of this bias. For example hourly average wind speeds are calculated by vector averaging of a series of lower frequency wind observations. A comparison of the hourly ending one minute wind speed with the hourly average wind speed may give some indication of the extent of the bias.

MODEL PERFORMANCE EVALUATION

The UAM(CB-IV) was exercised with the exact same inputs as in evaluation run 2 except with the a wind field in which the observed wind speeds from FAA observations were reduced by 50 percent. The resultant predicted ozone concentrations at each of the ozone monitoring sites are shown in Figure G-1. Similar time series plots of predicted and observed ozone concentrations using a one-cell and two-cell search are given in Figure G-2 and G-3. Scatterplots, residual analysis plots, and model performance statistics for predicted and observed hourly ozone concentrations and the reduced wind speed sensitivity test are shown in Figure G-4. The isopleths of hourly ozone concentrations for the reduced wind speed sensitivity test are given in Figure G-5. Note that these five figures correspond to Figures 3 through 6 in the main body of the report and Appendix E for evaluation run 2.

The predicted region-wide maximum ozone concentration in the reduced wind speed sensitivity test matches the observed peak ozone concentration exactly (14.7 pphm). At the location of the observed peak ozone the model prediction (11.4) is within 22 percent. At other ozone monitors the model predicts the peak within 2 (DKLB) and 33 (DLLS) percent. The reduced wind speed sensitivity test exhibits superior model performance over evaluation run 2 as exhibited in the scatterplots of hourly predicted and observed ozone concentrations (Figures G-4, and Figure 6 in the main body of the report).

VOC EMISSION REDUCTION SCENARIOS

The same three (30, 60, and 90 percent) across the board anthropogenic VOC emission reduction scenarios were performed using the reduced wind speeds sensitivity test model inputs as were performed using the evaluation run 2 modeling inputs. Table G-2 shows the effects of the VOC anthropogenic emission reductions on the predicted region wide maximum ozone concentrations with and without biogenic emissions. A graphical representation of the information from Table G-2 is presented in Figure G-7. Using the reduced wind speeds sensitivity test modeling inputs it is estimated that anthropogenic VOC emission reductions of 62 and 53 percent are required for the case of with and without biogenic emissions, respectively. Note that this is only a 9 percent increase in anthropogenic VOC emission reduction to reach attainment when including biogenics as compared to the 38 percent additional controls estimated when using the evaluation run 4 modeling inputs.

This difference in calculated VOC emission redeuction control requirements using the evaluation run2 and the sensitivity test modeling data base is not surprising because the reduced wind speeds in the sensitivity test mean that more of the ozone peak is due to the urban anthropogenic emissions. These differences do underscore the uncertainty in the model calculations, be they due to uncertainties in emissions (anthropogenic and biogenic), boundary conditions, or meteorology. Thus the emphasis on the findings reported here and elsewhere (e.g., Chameides et al., 1988) concerning biogenic emissions should be on the directions rather than the absolute magnitudes of the calculations. However, the reduced wind speed sensitivity test does not change the basic result that biogenic emissions in Atlanta do affect the amount of anthropogenic VOC emission reduction required to meet attainment of the ozone standard.

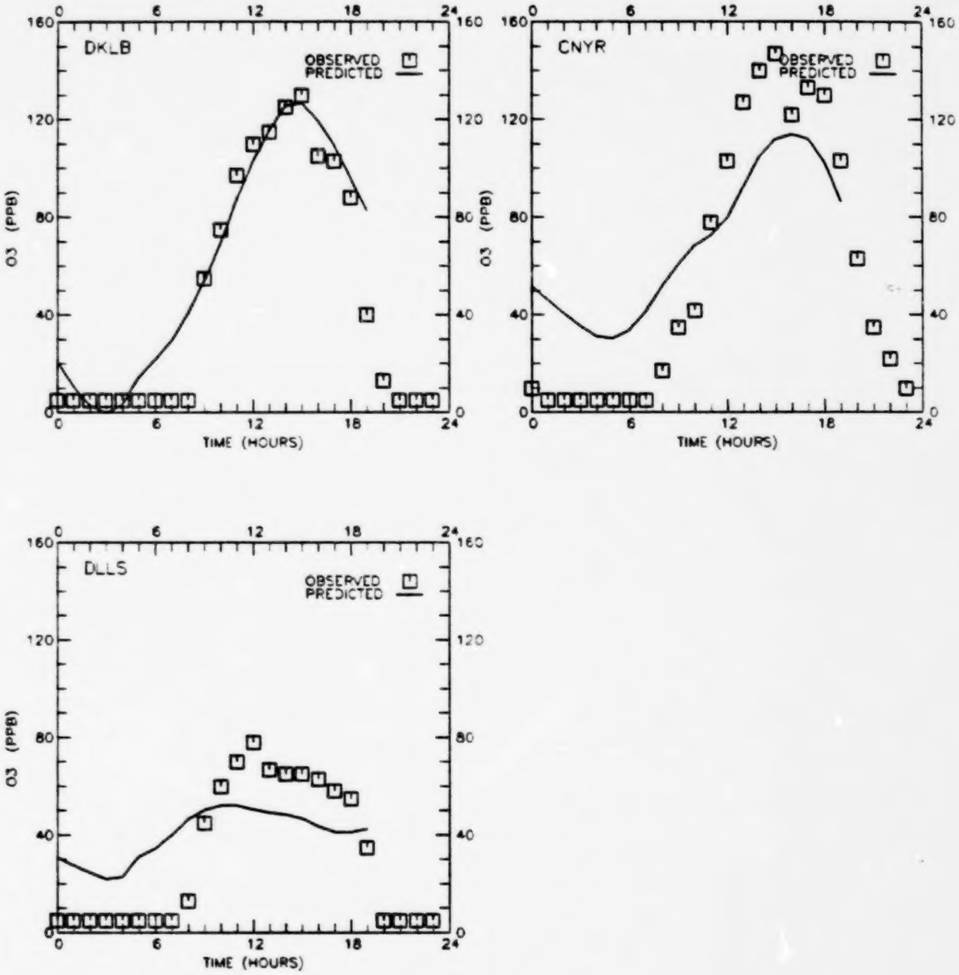
TABLE G-1. Surface meteorological observation sites and distance between collocated observations pairs.

NWS/FAA Site Name	Location UTM (Zone10)		SCAQMD Site Name	Location UTM (Zone 10)		Distance between Collocated Stations
	UTM$_x$	UTM$_y$		UTM$_x$	UTM$_y$	
Burbank Airport	356.48	3768.00	Burbank	359.60	3766.40	3.52 km
Los Angeles International Airport	352.48	3744.40	Lennox	354.40	3744.00	1.96 km
Long Beach Airport	370.88	3733.76	Long Beach	368.00	3734.40	2.95 km
El Toro Airport	401.60	3720.16	El Toro	404.8	3716.72	4.70 km
Ontario Airport	411.68	3754.16	Upland	408.00	3758.48	5.67 km
Norton Air Force Base	438.80	3756.96	San Bernardino	434.40	3759.20	4.94 km
Compton Airport	364.40	3740.24	Lynwood	366.40	3743.20	3.57 km

TABLE G-2. Regional maximum ozone concentrations (pphm) predicted by the UAM for the base cases (with and without biogenic emissions) and the different emission scenarios using the reduced wind speed sensitivity test modeling inputs.

	Maximum Ozone Concentration pphm	Percent Reductions from Base Case	Maximum Ozone Normalized to Peak Observation (pphm)
Peak Observed	14.7	0.0	14.7
Ozone NAAQS*	12.0	18.4	12.0
With Biogenics			
0% VOC Reduction	14.70	0.0	14.7
30% VOC Reduction	13.17	10.4	13.2
60% VOC Reduction	12.09	17.8	12.1
90% VOC Reduction	11.24	23.5	11.2
Without Biogenics			
0% VOC Reduction	12.93	0.0	14.7
30% VOC Reduction	11.83	8.5	13.5
60% VOC Reduction	10.09	22.0	11.5
90% VOC Reduction	8.82	31.8	10.0

* Technically, the ozone NAAQS is 0.12 ppm rounded. Thus, an ozone concentration of 12.4 pphm (15.6% reduction from observed peak) is considered attainment.



SYSTEMS APPLICATIONS, INC.

FIGURE G-1. Observed and predicted ozone concentrations (ppb) for Atlanta reduced wind speed sensitivity test.

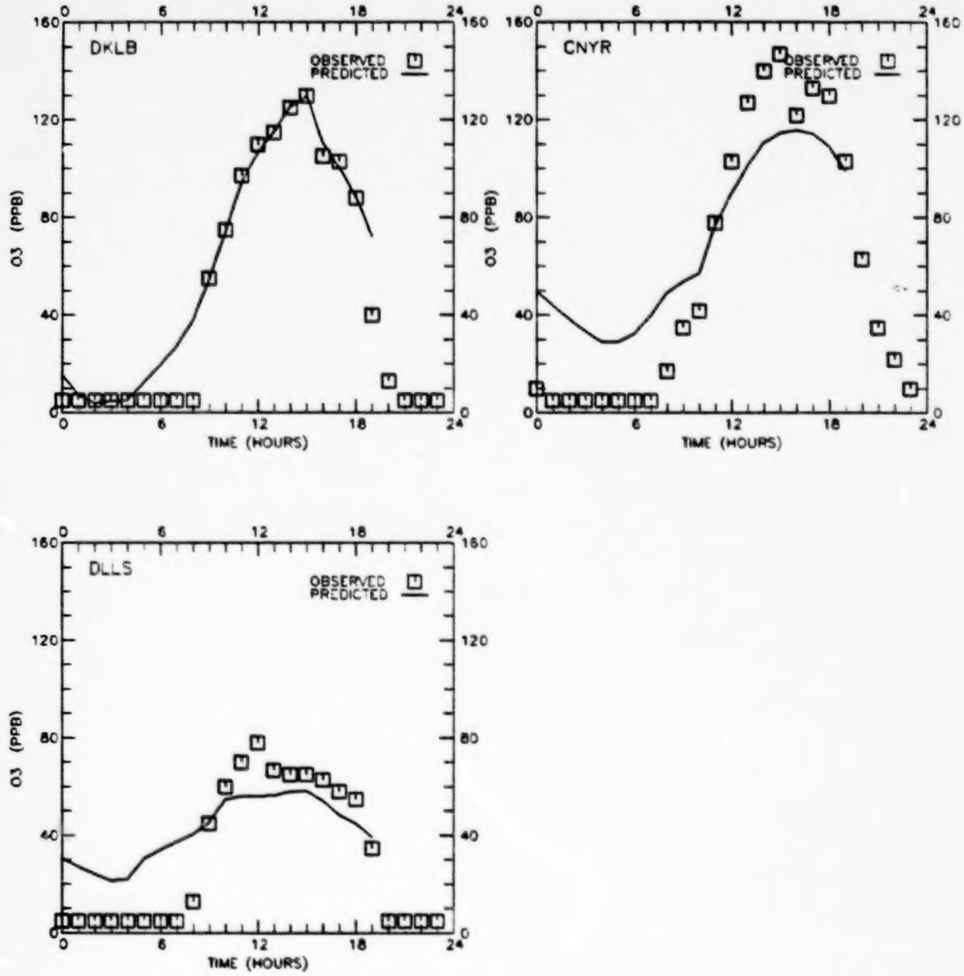
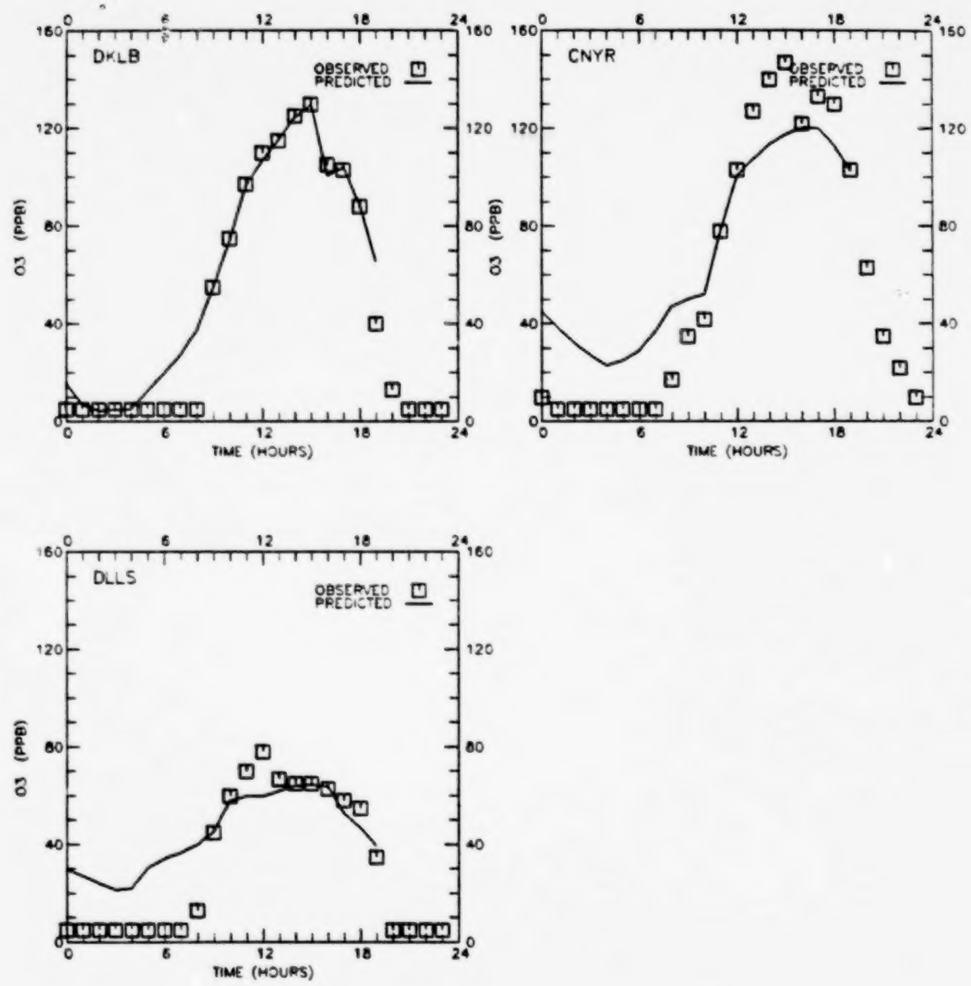
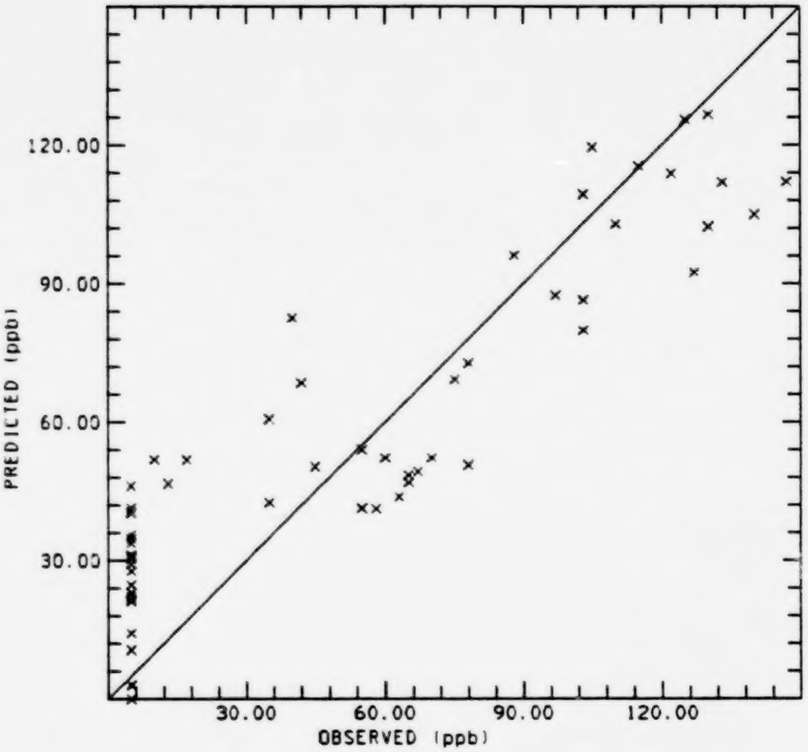


FIGURE G-2. Observed and nearest-neighbor predicted (one-cell search) ozone concentration (ppb) for the Atlanta reduced wind speed sensitivity test.



SYSTEMS APPLICATIONS, INC.

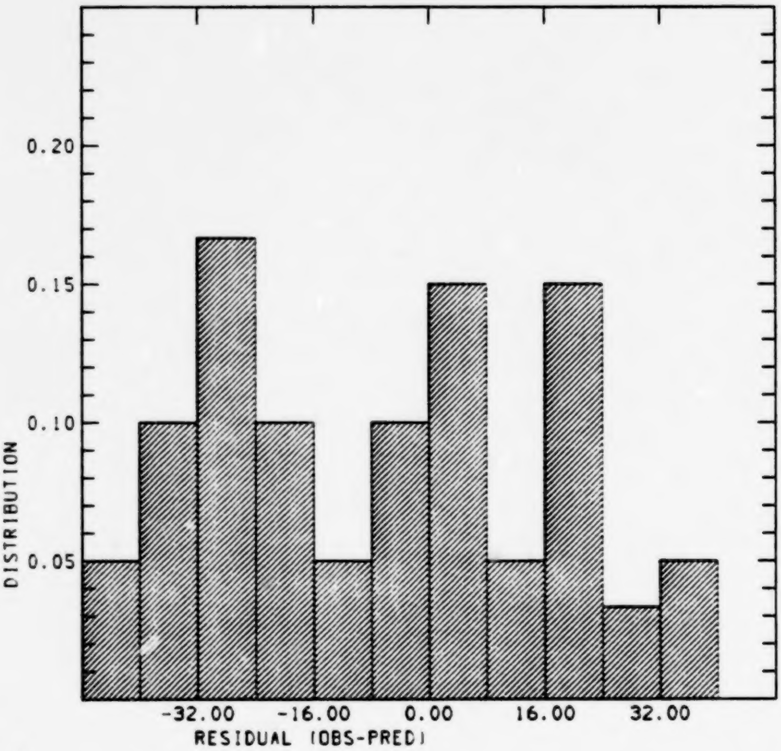
FIGURE G-3. Observed and nearest-neighbor predicted (two-cell search) ozone concentration (ppb) for the Atlanta reduced wind speed sensitivity test.



```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                        OBSERVED       PREDICTED
       AVERAGE          50.39999        56.68703
  STANDARD DEVIATION    47.63355        34.20863
       SKEWNESS         0.51320        0.52057
       KURTOSIS         -1.22432        -0.84048
   OTHER MEASURES
       MEDIAN           40.00000        46.90000
    UPPER QUARTILE      88.00000        82.56000
    LOWER QUARTILE      5.00000        31.13000
    MINIMUM VALUE       5.00000        0.02000
    MAXIMUM VALUE       147.00000        126.60000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED    0.904
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.844 HIGH BOUND 0.942
RATIO OF OVER TO UNDER PREDICTIONS  1.308
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED    41.667
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED    1.667
```

FIGURE G-4a. Scatterplot and model performance statistics for hourly ozone concentrations and Atlanta reduced wind speeds sensitivity test (N = 60).

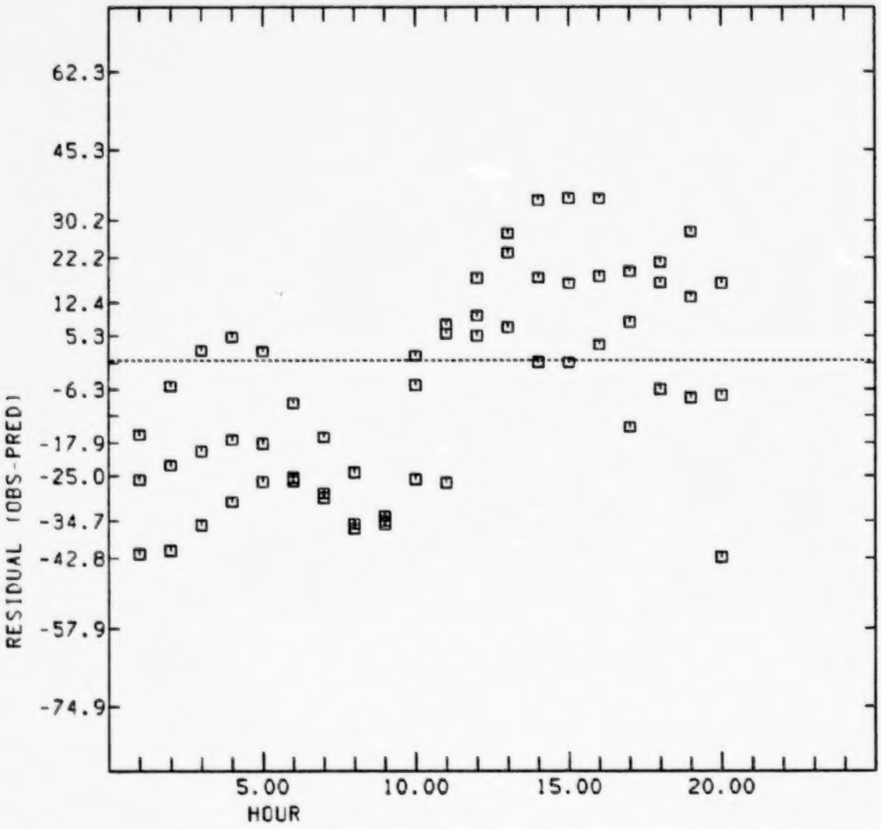


```
THE BINSIZE EQUALS  8.000
```

```
RESIDUAL ANALYSIS

          AVERAGE          -6.28719
  STANDARD DEVIATION       22.19390
         SKEWNESS          0.10702
         KURTOSIS          -1.19285
   OTHER MEASURES
          MEDIAN           -6.30000
     UPPER QUARTILE        9.57001
     LOWER QUARTILE        -26.13000
      MINIMUM VALUE        -42.56000
      MAXIMUM VALUE        35.00000
```

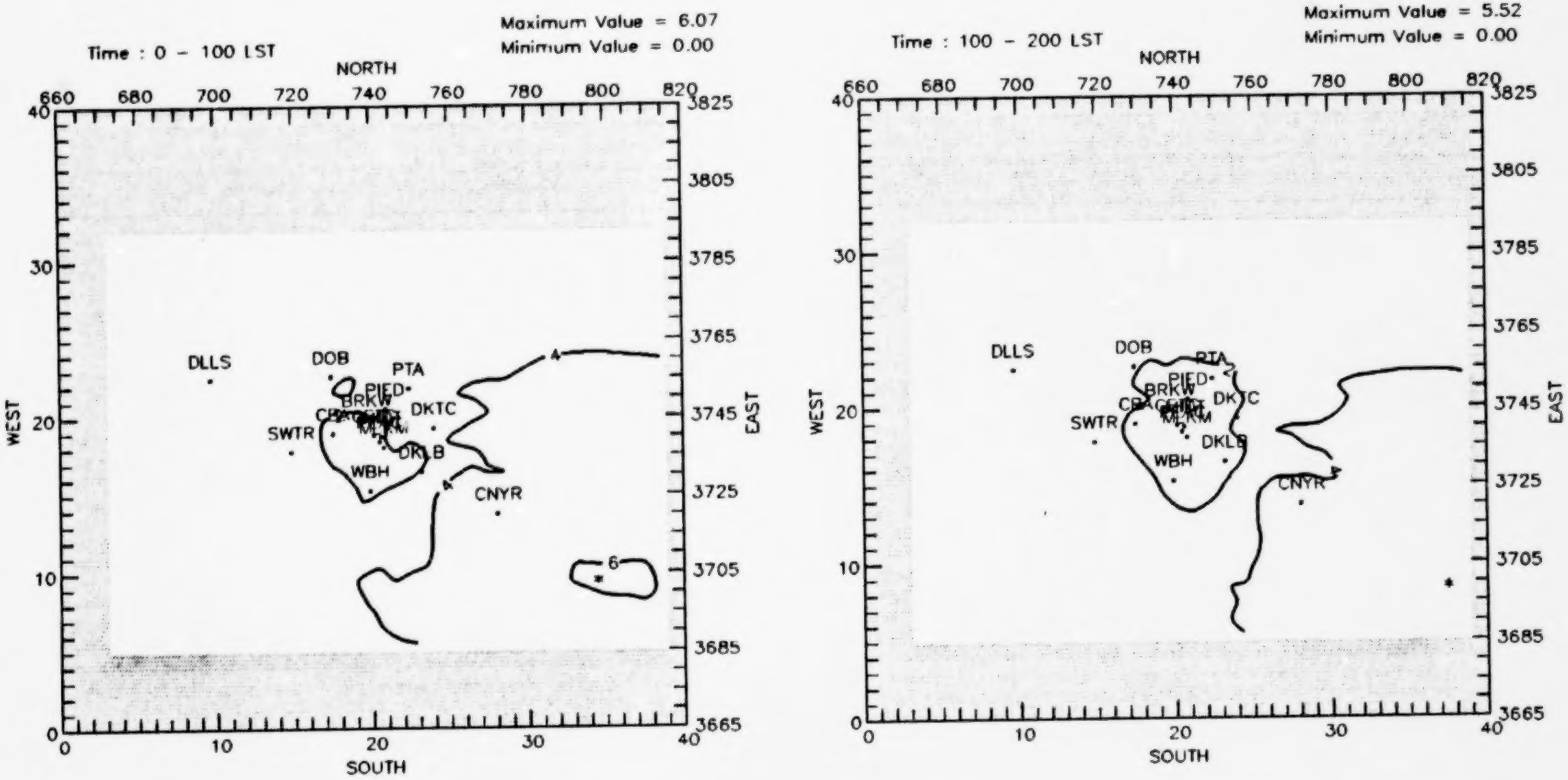
```
BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND -18.9385
UPPER BOUND 6.3641

STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 373.7107
UPPER BOUND 684.3732

THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 22.89
THE AVERAGE ABSOLUTE ERROR IS 19.52

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                                 0.9451
RESIDUAL COEFFICIENT OF VARIATION
                                 0.4404
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                 0.4659
```

FIGURE G-4b. Residual analysis plot and model performance statistics for hourly ozone concentrations and Atlanta reduced wind speeds sensitivity test.



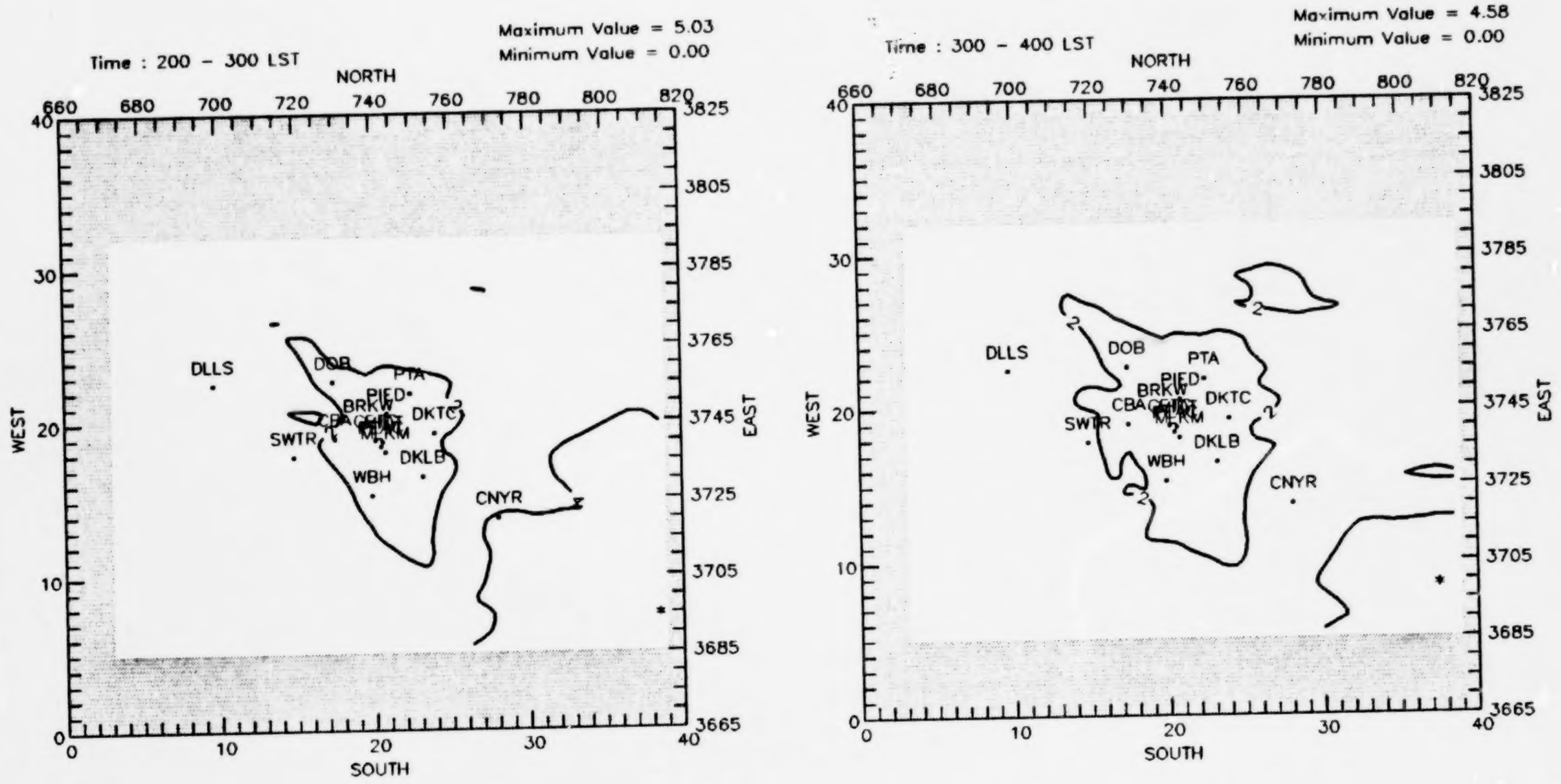
```
THE LINEAR MODEL PARAMETERS
THE CORRELATION IS 0.5829
THE LOWER BOUND IS 0.3861
THE UPPER BOUND IS 0.7290
AT THE 0.0500 PERCENT LEVEL
THE Y-X LINEAR MODEL INTERCEPT IS 11.460
THE Y-X LINEAR MODEL SLOPE IS 0.153
THE X-Y LINEAR MODEL INTERCEPT IS -29.647
THE X-Y LINEAR MODEL SLOPE IS 2.225
```

FIGURE G-4c. Plot of residuals versus time of day for hourly ozone concentrations and Atlanta reduced wind speeds sensitivity test.



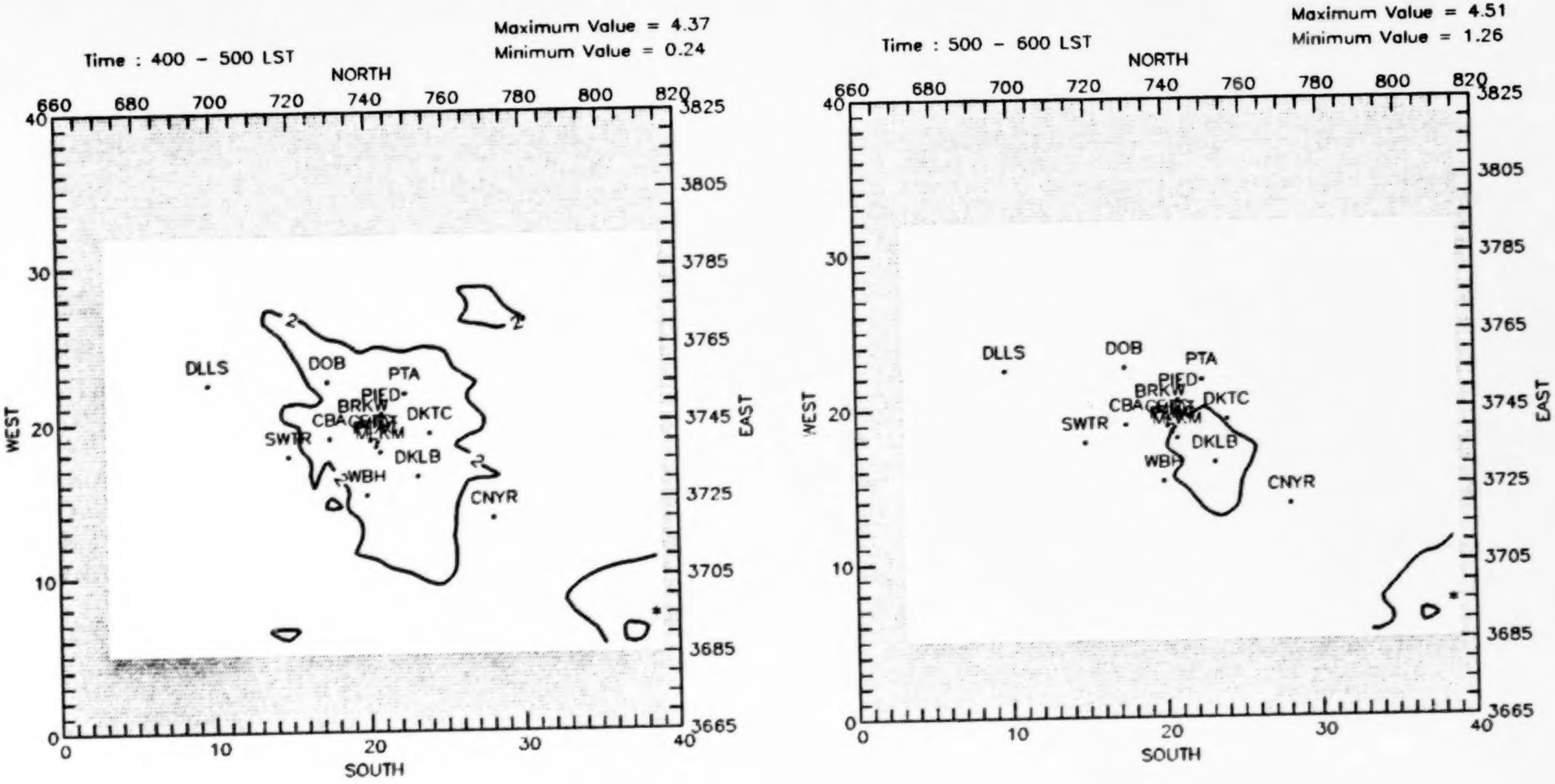
Time : 0 - 100 LST
Maximum Value = 6.07
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
DKTC
SWTR
DKLB
WBH
CNYR
4
6
Time : 100 - 200 LST
Maximum Value = 5.52
Minimum Value = 0.00

FIGURE G-5. Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm).


Time : 200 - 300 LST
Maximum Value = 5.03
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
2
Time : 300 - 400 LST
Maximum Value = 4.58
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
2

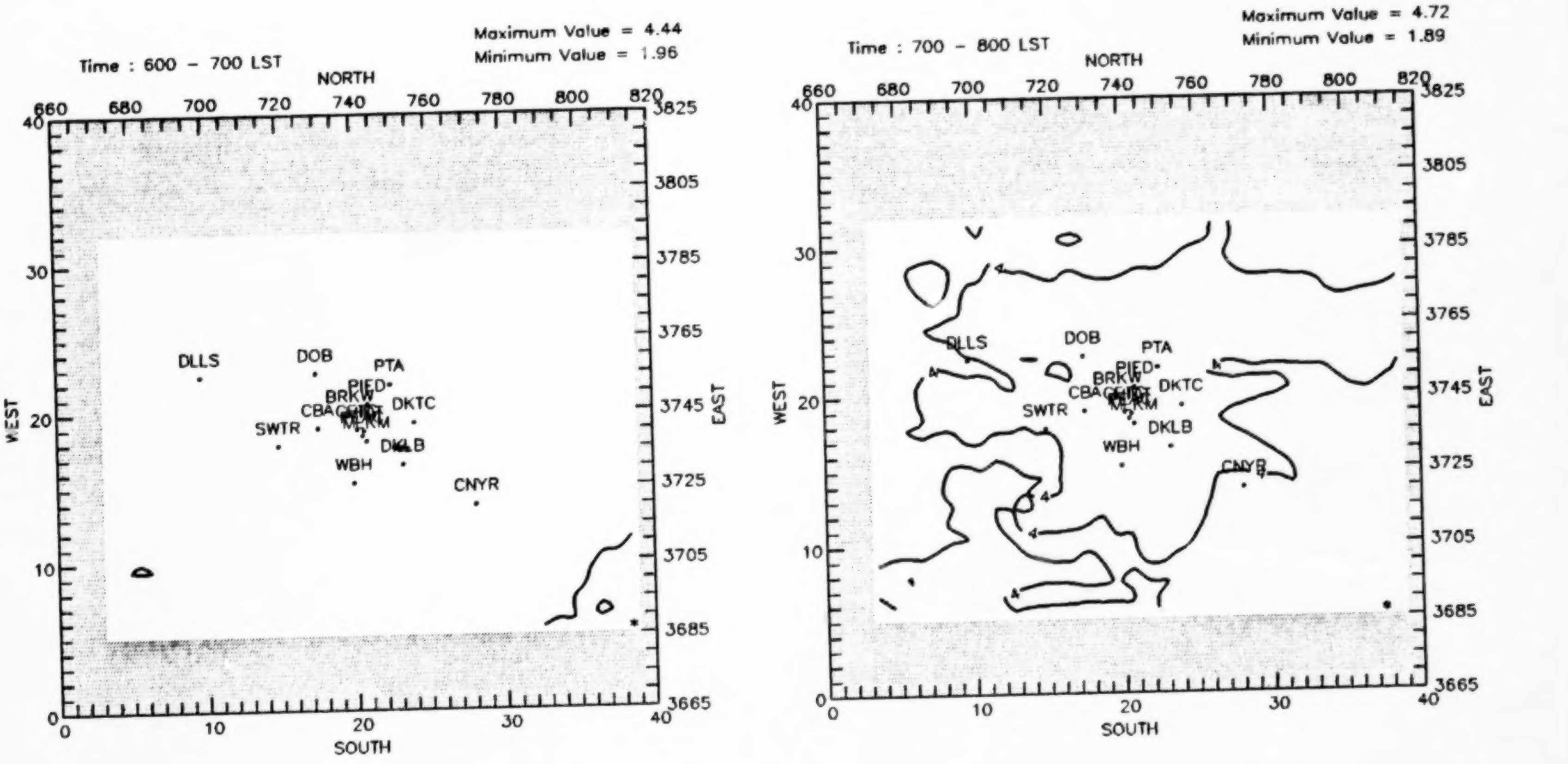
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.


Time : 400 - 500 LST
Maximum Value = 4.37
Minimum Value = 0.24
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
DKLB
WBH
CNYR
2
Time : 500 - 600 LST
Maximum Value = 4.51
Minimum Value = 1.26
NORTH
SOUTH
WEST
EAST
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
DKLB
WBH
CNYR

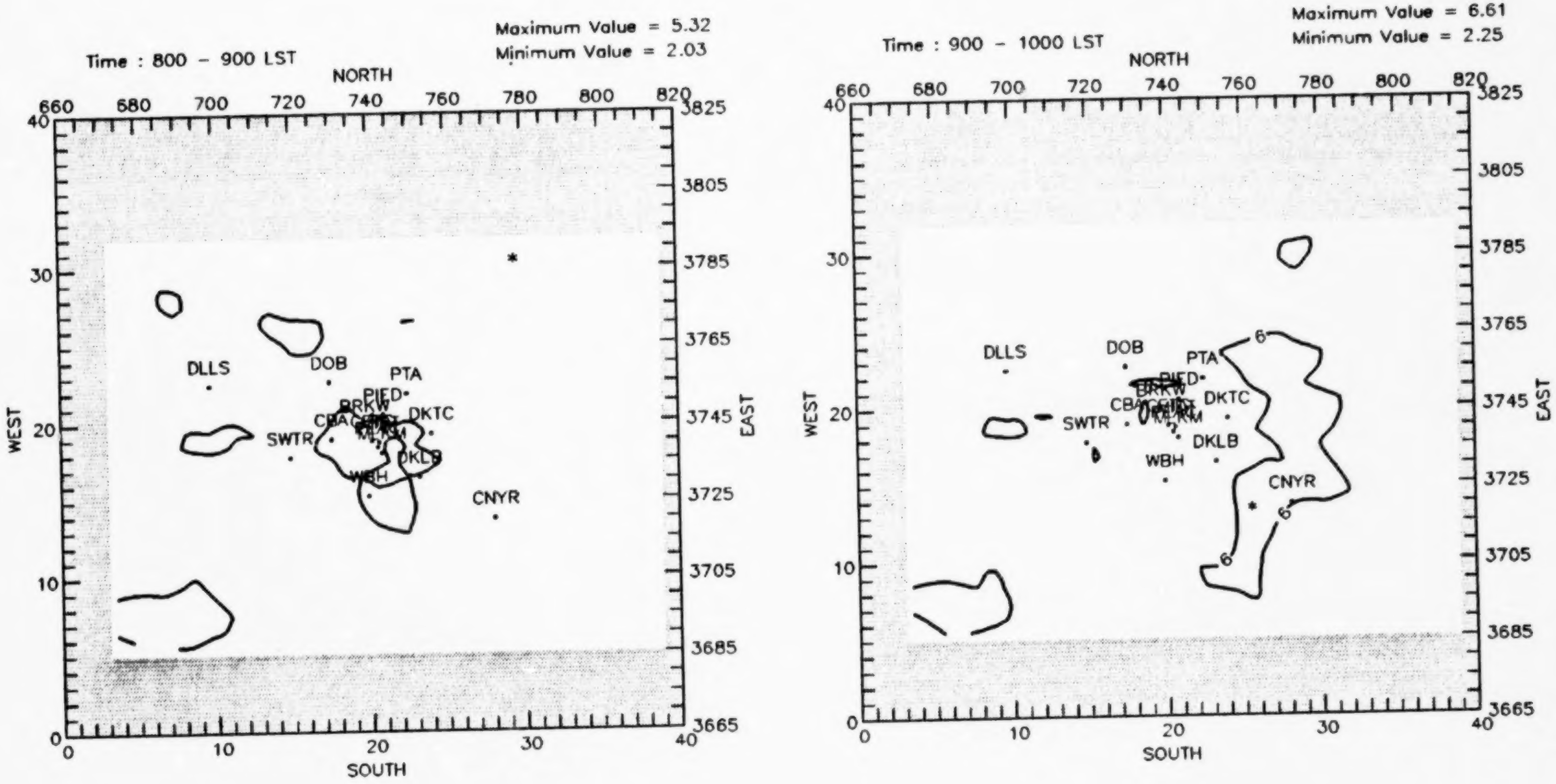
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.


Time : 600 - 700 LST
Maximum Value = 4.44
Minimum Value = 1.96
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
Time : 700 - 800 LST
Maximum Value = 4.72
Minimum Value = 1.89
4

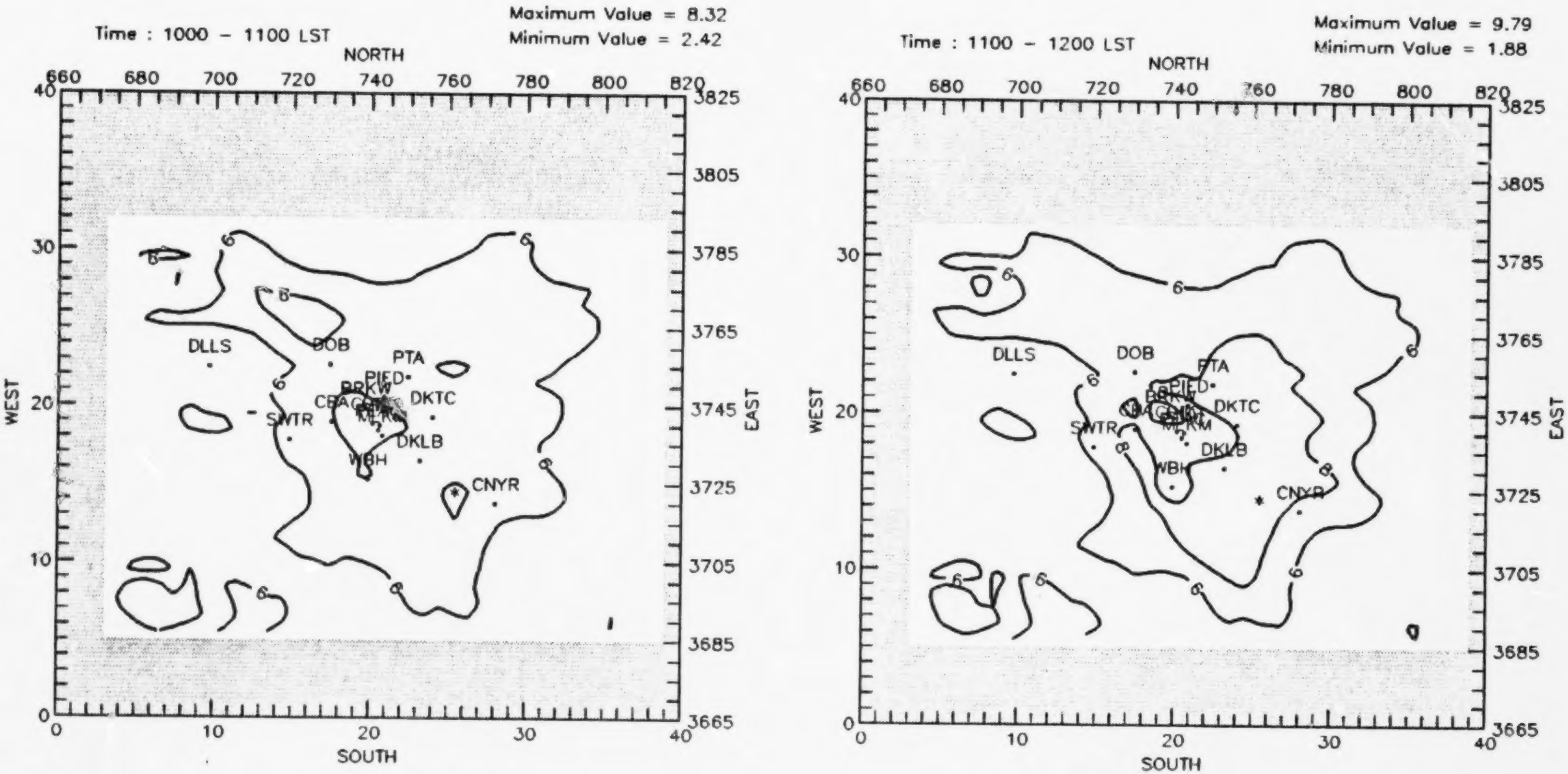
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.


Time : 800 - 900 LST
Maximum Value = 5.32
Minimum Value = 2.03
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
Time : 900 - 1000 LST
Maximum Value = 6.61
Minimum Value = 2.25
NORTH
SOUTH
WEST
EAST
DLLS
DOB
PTA
PIED
BRKW
CBA
DKTC
SWTR
MLKM
DKLB
WBH
CNYR
6

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.



Time : 1000 – 1100 LST

Maximum Value = 8.32
Minimum Value = 2.42

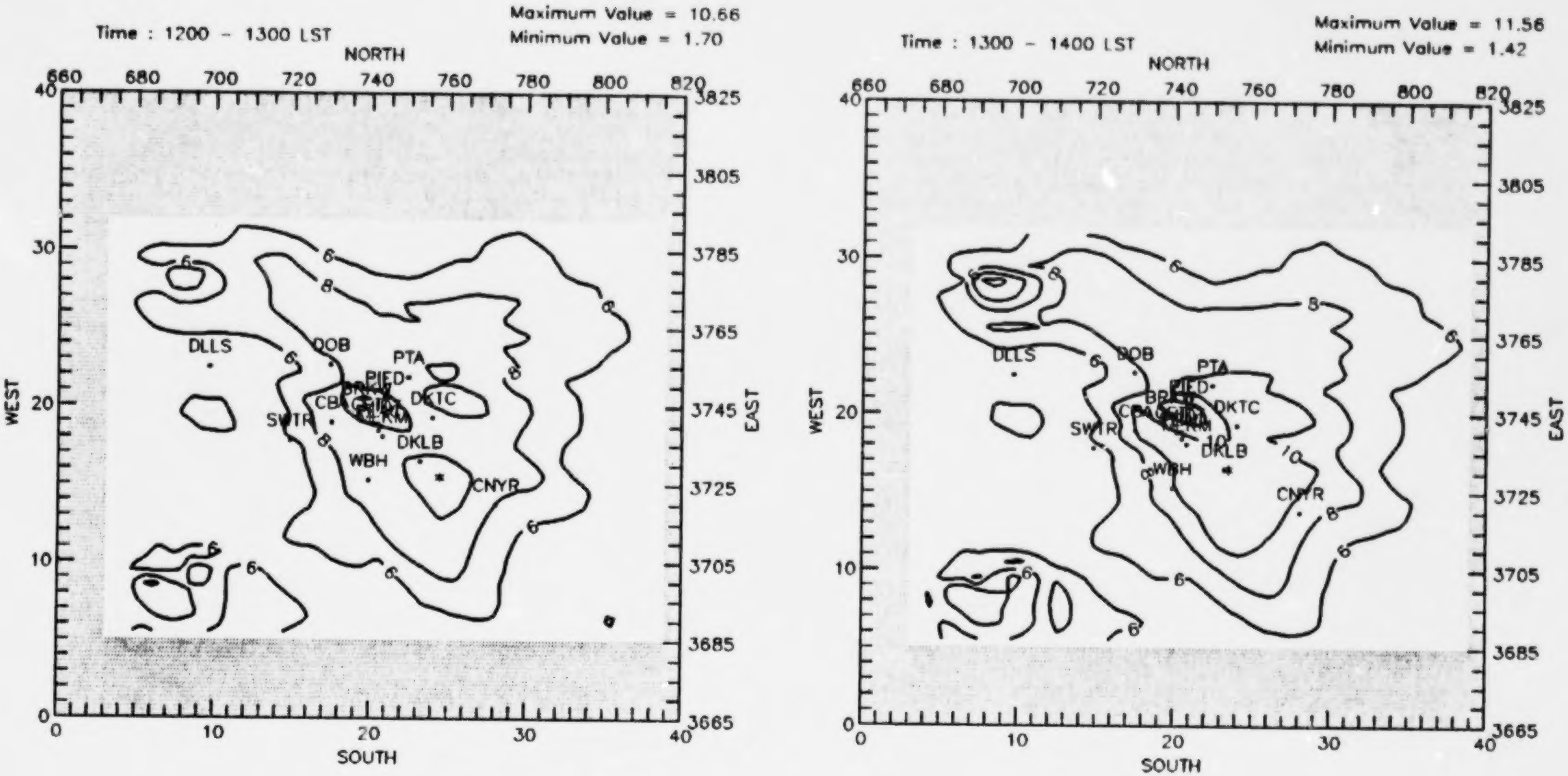
Time : 1100 – 1200 LST

Maximum Value = 9.79
Minimum Value = 1.88

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
6
8
DLLS
DOB
PTA
PIED
BRKW
CBAG
DKTC
SWTR
DKLB
WBH
CNYR
MLKM

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.



Time : 1200 - 1300 LST

Maximum Value = 10.66
Minimum Value = 1.70

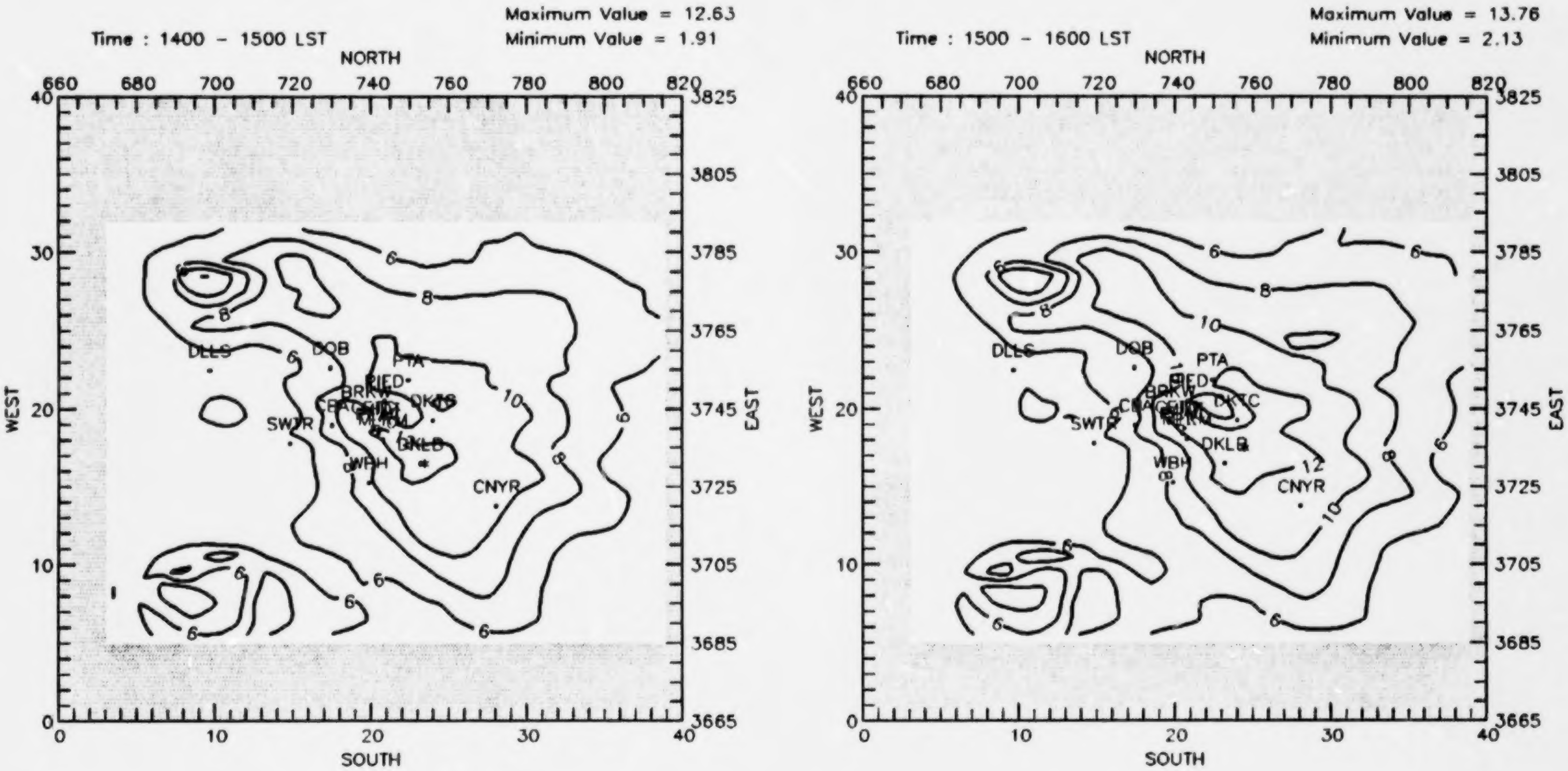
Time : 1300 - 1400 LST

Maximum Value = 11.56
Minimum Value = 1.42

NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
0
10
20
30
40
3825
3805
3785
3765
3745
3725
3705
3685
3665
DLLS
DOB
PTA
PIED
CBA
SWTR
DKTC
DKLB
WBH
CNYR
6
8
10

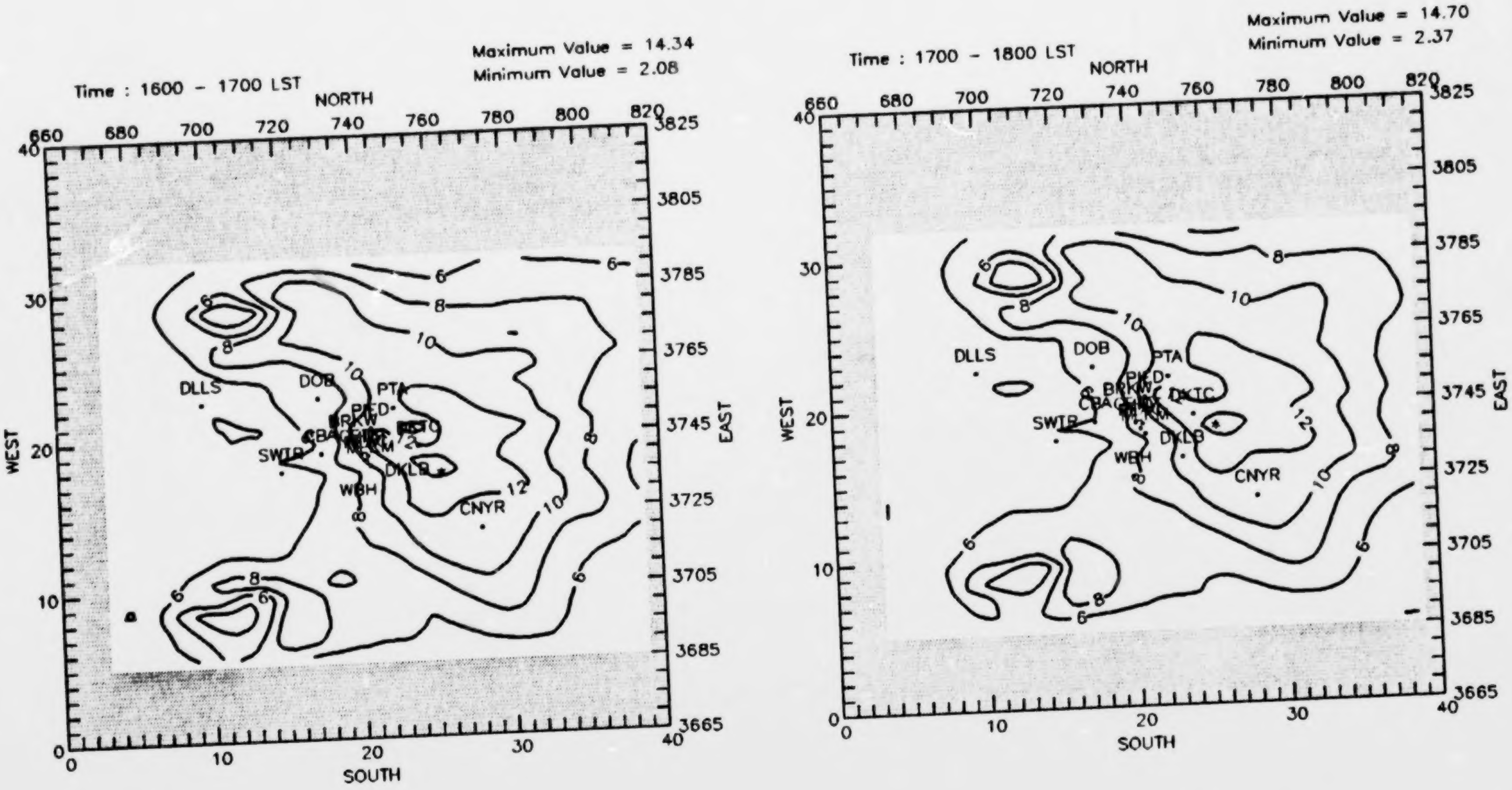
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.


Time : 1400 - 1500 LST
Maximum Value = 12.63
Minimum Value = 1.91
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
RIED
BRKW
CBA
DKTC
SWTR
WBH
DKLB
CNYR
6
8
10
Time : 1500 - 1600 LST
Maximum Value = 13.76
Minimum Value = 2.13
12

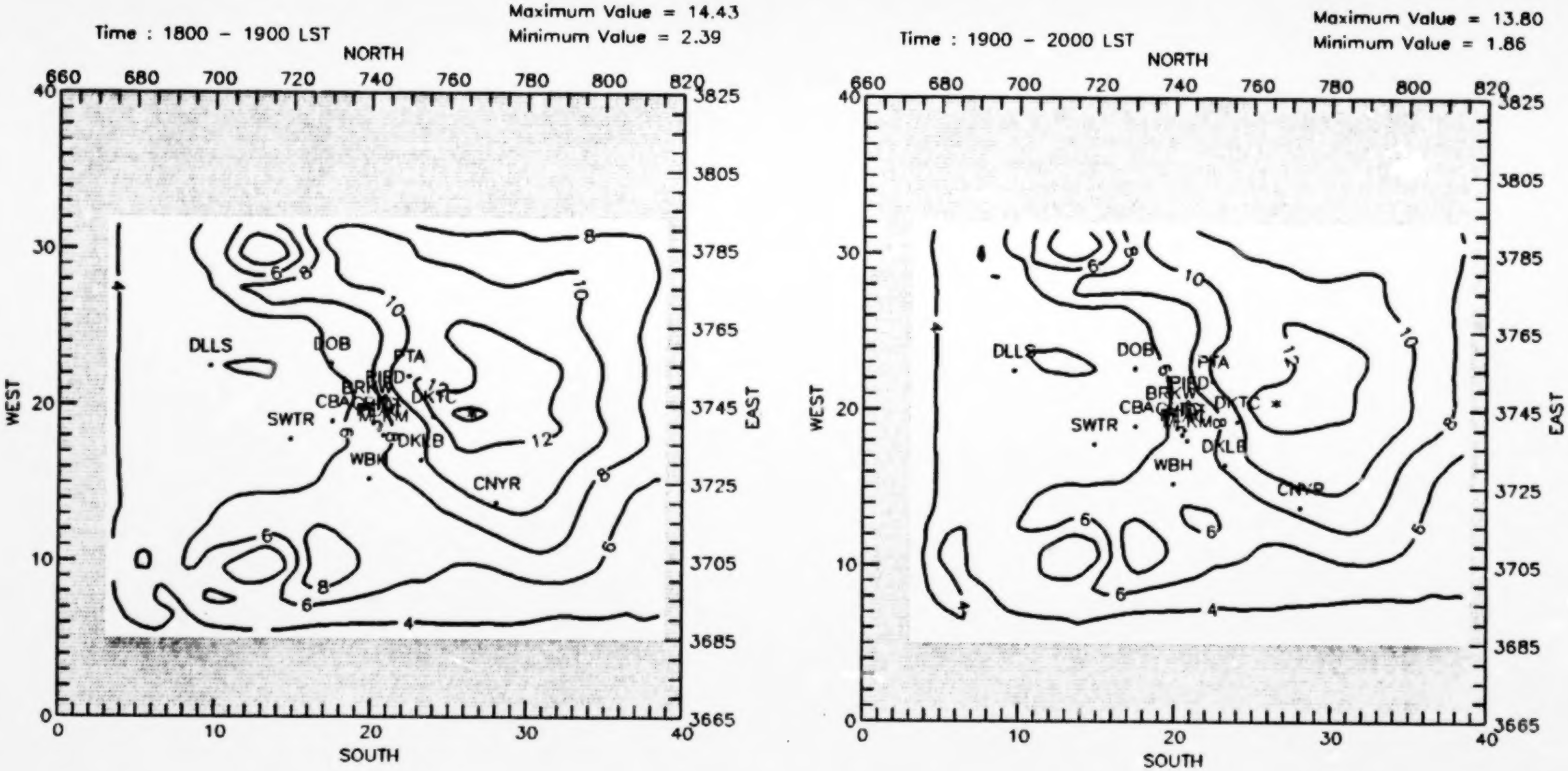
Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.


Time : 1600 - 1700 LST
Maximum Value = 14.34
Minimum Value = 2.08
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
PKED
BRKW
CBAG
SWIR
WBH
DKLB
CNYR
6
8
10
12
Time : 1700 - 1800 LST
Maximum Value = 14.70
Minimum Value = 2.37
DKTC

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Continued.


Time : 1800 - 1900 LST
Maximum Value = 14.43
Minimum Value = 2.39
NORTH
SOUTH
WEST
EAST
660
680
700
720
740
760
780
800
820
3825
3805
3785
3765
3745
3725
3705
3685
3665
0
10
20
30
40
DLLS
DOB
PTA
BRKW
PIRD
CBA
SWTR
DKTC
DKLB
WBH
CNYR
4
6
8
10
12
Time : 1900 - 2000 LST
Maximum Value = 13.80
Minimum Value = 1.86

Ozone (pphm) 1985 base emissions, June 4, 1984 (pphm)

FIGURE G-5. Concluded.

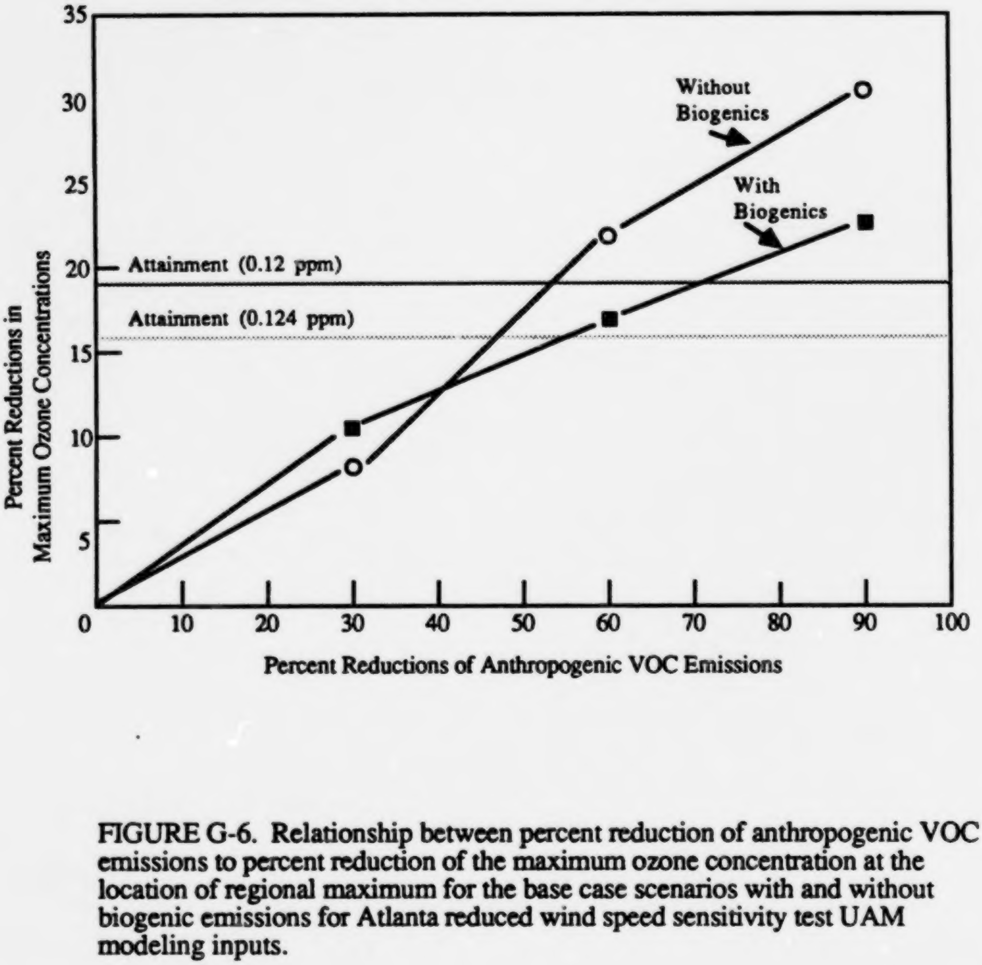


FIGURE G-6. Relationship between percent reduction of anthropogenic VOC emissions to percent reduction of the maximum ozone concentration at the location of regional maximum for the base case scenarios with and without biogenic emissions for Atlanta reduced wind speed sensitivity test UAM modeling inputs.

APPENDIX D

Biogenic VOC Chemistry Uncertainties

by

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March 1989

The chemistry of isoprene has been investigated by a number of scientists (Arnts et al. 1981, Gu et al. 1985, Grimsrud et al. 1975). The primary removal process for isoprene is through the reaction with OH radicals. At nighttime both O_3 and NO_3 react with isoprene. Since isoprene is, however, primarily emitted during the daylight hours, OH removal processes are the most important.

The most recent and extensive studies have been conducted by Atkinson et al. (1988). In this study, only about 50-60% of the carbon in isoprene can be accounted for. About 40-50% of the reaction pathways cannot be explained. The principal products observed were methacrolein, methyl vinyl ketone and formaldehyde. 3-Methyl furan was observed as a very minor product.

The CBM-IV used in both urban and regional models treats isoprene as a separate compound (Gery et al. 1988). The products, however, are not. Instead, the products are treated as species that are already used in the mechanism. Thus, the olefinic nature of the products are represented as ethene. The formation of PAN and PAN-type compounds from isoprene is represented by acetaldehyde and acetyl peroxyl radicals. Methyl glyoxal is used for the high radical yields.

The removal process for the terpenes have also been investigated (Schwartz, 1974, Arnts et al. 1981, Kaiserman et al. 1981, Grimrud et al. 1975). However, like isoprene, the carbon balances for the reacted terpenes are poor. In most cases only 10-40% of the carbon could be accounted for. Also, there appears to be some disagreement on the amount of aerosol produced. The latest work has obtained almost a complete carbon balance with the reaction of alpha-pinene with ozone (Hooker et al. 1985). This work used tagged carbon on only one carbon of the C_{10} olefin. Therefore, the carbon balance is obtained only for the tagged portion of the molecule. If a fraction of the molecule is fragmented, these experiments would not determine the carbon lost through fragmentation. Also, about 20% of the tagged carbon was observed on the walls of the reactor and there was no mechanistic description or identification of the material adsorbed on the walls.

CBM-IV does not treat alpha-pinene as a separate specie. It is treated as 0.5 OLE, 1.5 ALD2 and 6.0 PAR, all species that already exist in carbon bond mechanism. The obvious reason for this is that the chemistry of alpha-pinene and the terpenes in general is not well known.

Gery et al. (1988) have modeled the smog chamber data from UNC for both isoprene and alpha-pinene. Their data for the comparison between observed and calculated ozone values are shown in Table 1. It is noted that for isoprene, the average percent difference between predicted and measured ozone is ±23%. For alpha-pinene, the difference is greater, ±40%. The PAN and CH_2O fits are shown in Table 2 for both isoprene and alpha-pinene. As noted, the PAN fits for alpha-pinene are extremely poor with the calculated PAN almost always being greater than the observed. This is probably a result of the over-representation of the alpha-pinene with 1.5 ALD. For isoprene, the PAN concentrations fits do not appear to be any worst than for O_3. The position of the maxima, however, appear to be shifted (e.g. for July 14, 1980, the model predicts 0.118 ppm at 200 minutes while the measured is 0.101 at 500 minutes (see attached Figure 1)).

The fits for the formaldehyde are not much better for both isoprene and alpha-pinene. Even when the maxima are in reasonable agreement the times for the maxima do not always agree.

As noted above, the uncertainties in the chemistry of natural hydrocarbons are vast. Since only approximately 50% of the mechanism is known for isoprene and even less for the C_{10} terpenes the modelers probably had no recourse but to parameterize the compounds as Gery et al. did. It is, therefore, not surprising that there is disagreement between the model predictions and the measured values. This is especially true with the PAN chemistry and its effect on ozone formation for the second day. Also, since PAN concentrations are very temperature-dependent, the amount of PAN predicted may not compare favorably with the measured values at different temperatures. An example of this can be seen by comparing the data of June 17, 1980 with those of July 17, 1980. In June, the maximum temperature reached was 303°K. In July, the temperature was 311°K. The model overpredicts PAN in June while it underpredicts PAN in July.

It is presently not known if the model is a poor representation of the actual degradation pathways or if the experimental data are poor. Formaldehyde and PAN are very difficult compounds to measure and there is always the possibility that the experimental data for these compounds are in error. The modeling efforts of Gery et al. are probably the best available in describing the photooxidation of natural hydrocarbons. Unless more data are obtained for these compounds, it is highly doubtful that the modeling efforts will improve.

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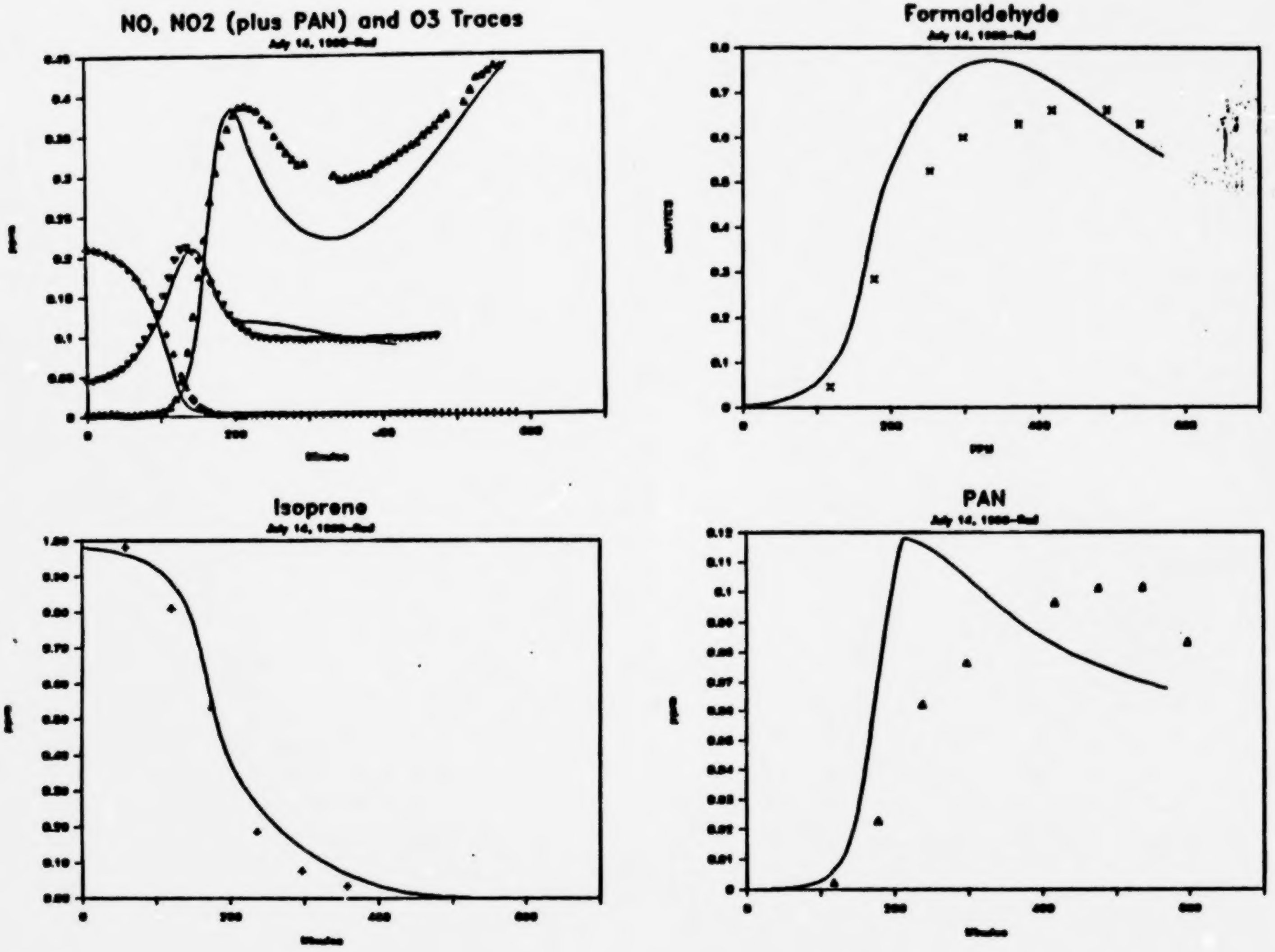

Figure 1. **Simulation results for UNC experiment JL1480R (symbols are experimental measurements)**

Table 1. Result of UNC Isoprene and α-Pinene Simulations

Experiment Number	Initial Conditions			Maximum Ozone (ppm)			
	NO_x	NO_2/NO_x	HC/NO_x	Calc. (ppm)	Meas. (ppm)	Abs. Diff.	Pct. Diff.
Isoprene:							
JL1480B	0.243	0.169	8.9	0.730	0.630	0.100	15.9%
JL1480R	0.255	0.173	19.2	0.475	0.435	0.040	9.3%
JL1680B	0.186	0.226	10.6	0.748	0.837	-0.089	-10.6%
JL1680R	0.180	0.239	22.4	0.502	0.652	-0.150	-23.0%
JL1780B	0.460	0.174	5.6	0.959	1.297	-0.338	-26.1%
JL1780R	0.466	0.161	2.1	0.725	0.806	-0.081	-10.0%
JN1780B	0.096	0.219	13.5	0.363	0.406	-0.043	-10.6%
JN1780R	0.189	0.275	2.6	0.479	0.354	0.125	35.3%
JN2080R	0.478	0.205	1.0	0.130	0.088	0.042	47.7%
JN2280B	0.205	0.146	7.6	0.658	0.550	0.108	19.6%
JN2280R	0.203	0.143	18.9	0.434	0.392	0.042	10.7%
JN2380B	0.210	0.181	6.0	0.665	0.570	0.094	16.5%
			Isoprene Average			-0.013	6.3%
			Std. Deviation			±0.136	±22.8%
α-Pinene:							
JL2580B	0.247	0.198	3.8	0.274	0.334	-0.060	-18.0%
JL2580R	0.247	0.162	4.1	0.340	0.377	-0.037	- 9.8%
JN1580B	0.219	0.192	3.7	0.309	0.332	-0.023	- 6.9%
JN1580R	0.213	0.207	5.7	0.572	0.473	0.099	20.9%
JL1580B	0.188	0.165	14.3	0.573	0.470	0.103	21.9%
JL1580R	0.184	0.163	5.7	0.425	0.202	0.223	110.4%
JN1480B	0.212	0.142	8.0	0.564	0.519	0.045	8.7%
JN1480R	0.210	0.133	15.0	0.552	0.465	0.087	18.7%
JN2180R	0.499	0.210	3.9	0.363	0.223	0.140	63.2%
			α-Pinene Average			0.064	23.2%
			Std. Deviation			±0.092	±40.5%
			Biogenic HC Average			0.020	13.5%
			Std. Deviation			±0.123	±31.9%

Table 2. Results of UNC Isoprene and α-Pinene Simulations

	Maximum PAN (ppm)				Maximum HCHO (ppm)			
Experiment Number	Calc. (ppm)	Meas. (ppm)	Abs. Diff.	Pct. Diff.	Calc. (ppm)	Meas. (ppm)	Abs. Diff.	Pct. Diff.
Isoprene:								
JL1480B	0.120	0.101	0.019	19%	0.379	0.381	-0.002	- 1%
JL1480R	0.118	0.101	0.017	17%	0.772	0.660	0.112	17%
JL1680B	0.086	0.080	0.006	8%	0.357	0.346	0.011	3%
JL1680R	0.082	0.072	0.010	14%	0.643	0.548	0.095	17%
JL1780B	0.168	0.188	-0.020	- 11%	0.452	0.633	-0.181	- 29%
JL1780R	0.035	0.047	-0.012	- 26%	0.194	0.230	-0.036	- 16%
JN1780B	0.058	0.053	0.005	9%	0.203	0.182	0.021	12%
JN1780R	0.039	0.034	0.005	15%	0.091	0.076	0.015	20%
JN2080R	0.006	0.008	-0.002	- 25%	0.099	-	-	-
JN2280B	0.109	0.086	0.023	27%	0.269	0.374	-0.105	- 28%
JN2280R	0.106	0.069	0.037	54%	0.607	0.572	0.035	6%
JN2380B	0.099	0.081	0.018	22%	0.224	0.196	0.028	14%
Isoprene Average			0.009	10%			-0.001	1%
Std. Deviation			±0.016	± 22%			±0.083	± 18%
a-Pinene:								
JL2580B	0.016	-	-	-	0.059	-	-	-
JL2580R	0.025	-	-	-	0.068	-	-	-
JN1580B	0.013	0.016	-0.003	- 19%	0.051	0.038	0.013	34%
JN1580R	0.049	0.022	0.027	123%	0.073	0.066	0.007	11%
JL1580B	0.128	0.033	0.095	288%	0.134	0.105	0.029	28%
JL1580R	0.048	0.011	0.037	336%	0.058	0.054	0.004	7%
JN1480B	0.096	0.032	0.064	200%	0.085	-	-	-
JN1480R	0.143	0.046	0.097	211%	0.236	-	-	-
JN2180R	0.054	-	-	-	0.103	-	-	-
α-Pinene Average			0.053	190%			0.013	20%
Std. Deviation			±0.040	±126%			±0.011	± 13%
Biogenic HC Average			0.024	70%			0.003	6%
Std. Deviation			±0.033	±112%			±0.071	± 18%